

Validation documentation
BR APIs & excipients, liquid/semi-solid (other)

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Introduction

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

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

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

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

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

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

Context of this document

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

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

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

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

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

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

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

Criteria for the inclusion of substances

This validation documentation describes the results of the validation of the reference database for the substance class *BR APIs & excipients, liquid/semi-solid (other)*. Validation documentation is created for each published version of the reference database for all substance classes incorporated.

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

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

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

- Any positive result of *Apo-Ident* confirms the identity of the substance/substance group and distinguishes it from all other substances of the database. In the case of substance groups, the result is ambiguous: Distinction from all substances not belonging to the group is proven. The substance is identified as a member of this group. However, within the substance group, it is not possible to reliably classify which substance has been tested.
- The criteria for clear identifiability are a [specificity](#) of 100 % ([true negative rate](#)) and a minimum distance in the distance matrix. See 2. d) under [Model creation procedure and validation runs](#) (for *cannabis flowers*, see [Appendix H](#)).

Validation concept

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

1. Collection of spectra for the *calibration sample*. The results (identities) of the calibration sample must be known. The calibration samples must be representative for the samples which are to be evaluated later. Therefore, they must take the various possible (physical) compositions into account. (Therefore, sourcing calibration samples for NIR from the specialist trade is superior to the use of CRS reference substances.)
2. The first mathematical step is *calibration*. Here, the [chemometric model](#) is calculated from the *calibration sample spectra* ([reference spectra](#)) and limits as well as some parameters are stipulated. The chemometric model is used later to calculate the analysis result (*prediction*).
3. Collection of further spectra for the *validation sample* which should be independent of the *calibration sample*. The results (identities) of the *validation sample* must also be known. The textbook suggests a random sample with a normal scope of 25 % to 50 % of the *calibration sample* [8].
4. The second technical data step is *validation*. Here, the [chemometric model](#) created is evaluated based on the spectra of the *validation samples*. As validation parameters for the identification, the *Ph. Eur. Section 2.2.40* [3] specifies the [specificity](#) and [robustness](#).

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

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

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

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

Model creation procedure and validation runs

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

1. Collecting the reference spectra (calibration sample)

- a) Procurement of the samples from the same sources from which pharmacies source their raw material for compounding (Caelo, Fagron, Euro-OTC, . . . , see also *DAC III.2. Bezugsquellen-nachweis für Rezepturbestandteile* [Sources of supply for compounding] [7]).
- b) Testing the suitability according to *ApBetrO* [Pharmacies Rules and Regulations] §§ 6, 11, that is to say the availability of a valid manufacturer certificates via identity, purity and contents of the batch.
- c) Recording standard 40 spectra of the sample in different positions, as a standard on four instruments. Here, handling and presentation of the samples as later in the pharmacy.
- d) Visual checking for anomalies in the spectra. In case of indications of measurement errors, measurement must be repeated. If a signature is missing in the spectrum, the substance may be excluded from the start as not promising (the spectra are nonetheless entered in the database validation as independent *Type B* spectra).
- e) Testing identity. For each substance, a certificate of correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the respective following substance page of this validation documentation the *Mahalanobis distance* to this reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance. Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

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

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

2. Generating the chemometric models (calibration)

- a) Determination of the transformation matrix from the reference spectra using variance maximisation [8, 9]. (*All* reference spectra are always included, even if only a few spectra are added for an update.) All reference spectra receive the same data pre-treatment, which is also later applied to all measurement spectra in the field (in the pharmacies).
- b) Checking that the number of principal components used is still sufficient.
- c) Calculating the limits for each substance from the spread of the reference spectra. The calculation regulation is identical for each substance in a substance class.
- d) Checking the distances between the limits of the separable substances: The distance matrix contains the *Mahalanobis distances* from each substance to each other. The values in a bidirectional manner are different in each case because the spread of the initial substance is included. If a distance is smaller than the minimal distance, the substances are not considered to be reliably separable. The minimal distance is set at 9. The developer of the model may specify a larger minimal distance (one value for the entire *chemometric model*), to increase the selectivity.
- e) Verification of the model using the reference spectra. No *false-positive* results are permitted.
- f) If one of the criteria is violated (d) *Minimum distance between two substances undershot* or (e) *One substance is identified as another*, the database developers decide which of the following options to apply:

- They remove both substances from the database. (The spectra remain in the validation and may also be included when generating the model. However, they are not offered for testing.)
 - They form a substance group of several substances which cannot be reliably separated. The result is then ambiguous: The chemometric model determines that the sample is one of the substances in the group and not another substance. However, it cannot determine which of the group members it is. In order to determine the clear identity, the user must carry out a suitable additional analysis.
 - They create another *chemometric model* with a smaller scope, in which at least all substances of the non-separable substance group are included (second-stage model). Second-stage models are only called up if the first stage has established that only one of the substances included in the second-stage model can be involved.
- g) If *chemometric models* that fulfil both criteria (distance matrix and no *false positives*), are available for all substance classes, they are combined with the evaluation algorithms to form an *IdentModule* and encoded. This unit can no longer be changed. Its overall function is checked by the validation.

3. Set of validation spectra (validation samples)

The following is provided for validation:

- a) *Type A*: The reference spectra = calibration spectra from which the database was generated. These also include spectra from substances which the *chemometric model* should not identify, but were also recorded during generation in order to increase selectivity. (As a result, the model “learns” to differentiate from other substances which are actually unknown to it.)
- b) *Type B*: Spectra recorded under the control of *HiperScan GmbH* and not used for the generation of the database. These also include reference spectra of other substance classes, and spectra that are not used as reference spectra. Samples are considered to be independent, if they originate from a batch, of which no spectra have been used for the generation of the database. (Up to *IdentModule 2018-01*, samples were still considered independent if the sampling was done independently, i.e. if they originate from another sales container.)
- c) *Type C*: Spectra from the field, which have not been recorded under the control of *HiperScan GmbH* and have not been used for the generation of the database. The spectra include not only substances of the substance class to be tested, but also substances from other classes.

All manufacturers’ batches from which spectra are used for the validation are listed by substance in this document: for substances included in the substance class *BR APIs & excipients, liquid/semi-solid (other)* in the respective validation reports; otherwise in attachments *A*, *B* and *C*.

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

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

4. Validation runs and approval

- a) Validation spectra are transferred holistically to the *IdentModule* for evaluation in the same way as the spectroscopy software *QuickStep* transfers measured spectra.
- b) Following the provision of each spectrum, the *IdentModule* responds as to whether it has recognised a substance and which substance was recognised.
- c) The correctness of this response is checked for each possible initial assumption (each measurable substance with the substance class) and counted according to *true negative*, *false negative*, *true positive* and *false positive*. These figures are provided for each substance and additionally in the section *Summary*, separated according to types *A*, *B* and *C*.

- d) No *false positive* results whatsoever are permissible.
- e) If the criterion is also met for all substance classes, the *IdentModule* is approved.

Particularities of individual substance classes

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

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

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

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

Significance of testing with *Apo-Ident*

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

Verbally, the statement of the analysis result can be expressed as follows. Here "*the spectra match*" means that the criteria *Mahalanobis distance*, *outlier analysis* and *correlation* are met as shown in *Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident* [4]. "The spectra do not match", on the other hand, means that at least the criterion *Mahalanobis distance* is not met. A different evaluation procedure is only used for *cannabis flowers* (see [Appendix H](#)).

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

1. The spectrum of the sample measured matches spectra of the defined substance.
2. The spectrum of the sample measured does not match any spectrum of any other substance in this substance class. Therefore, all other substances can be clearly ruled-out.
3. As the spectra from other substance classes were used for validation, it is proven that no spectrum of one of these other substances matches the defined substance. (All substance classes with which a spectrum comparison is possible and makes sense are used for validation. This is documented for each substance class in the section [Summary](#).)

4. If the defined substance belongs to a *substance group* which in itself is not clearly separable with *Apo-Ident*, matching with the spectra of one or several substances in this group is confirmed. Which of these substances it actually is cannot be determined clearly. All other substances are excluded analogous to 2 and 3.

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

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

Conclusion

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

Explanation of terminology

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

with r_p as the total number of *true positive* classifications and f_n as the total number of *false negative* classifications. The *true positive rate* is a measure for the recognition rate of the validated *Apo-Ident IdentModule*.

In order to ensure that each substance is received with the same weight, the spectra are weighted as described for the [true negative rate](#).

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

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

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

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

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

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

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

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

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

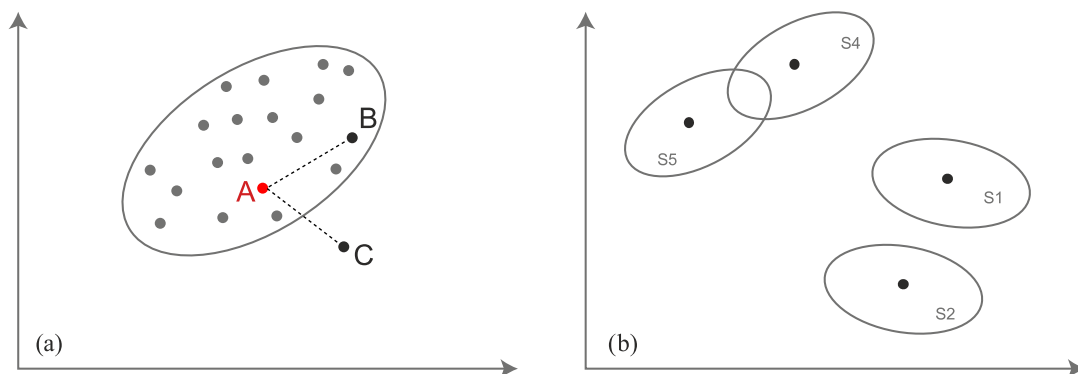


Figure 1: (a) The *Mahalanobis distance* from *A* to *B* is less than from *A* to *C*. However, the Euclidean distances are identical. (b) The *Mahalanobis distance* between the two measurement series *S4* and *S5* is smaller than between *S1* and *S2*. However, the Euclidean distances are identical.

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

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

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

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

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

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

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

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

Summary

A total of 88 261 spectra from 7522 different batches for a total of 215 substances were used to validate the substance class *BR APIs & excipients, liquid/semi-solid (other)*.

Validation samples

The validation samples can be categorised as follows:

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

Substance class	Substances	Batches	Spectra
APIs & excipients, liquid/semi-solid (other)	144	603	30 134

From category *A* a total of 30 134 spectra from 603 batches for a total of 144 substances were taken into account for validation.

Type B Spectra from independent samples which are not included in database generation. These spectra were recorded under the control of *HiperScan GmbH*. Detailed information regarding the batches or samples can be found in the following validation reports in the section *Type B* or in [Appendix B](#).

Substance class	Substances	Batches	Spectra
APIs & excipients, liquid/semi-solid (other)	211	710	32 090

From category *B* a total of 32 090 spectra from 710 batches for a total of 211 substances were taken into account for validation.

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

Substance class	Substances	Batches	Spectra
APIs & excipients, liquid/semi-solid (other)	167	6469	26 037

From category *C* a total of 26 037 spectra from 6469 batches for a total of 167 substances were taken into account for validation.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	19 975	0	1 935 405
Type B	0	15 560	625	2 147 289
Type C	0	12 159	90	1 441 955

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

	Specificity	Recognition rate
Type A	100.000 00 % (> 99.999 45 %)	100.000 00 % (> 99.955 88 %)
Type B	100.000 00 % (> 99.999 38 %)	94.729 88 % (> 94.689 98 %)
Type C	100.000 00 % (> 99.986 65 %)	98.563 15 % (> 98.005 42 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Angelica root oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30535-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Angelica root oil; Oleum angelicae (e radice)

Special notes

When selecting the *Angelica root oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Angelica root oil	6	3	8

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Angelica root oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Swiss pine oil	11.73	—
Camphor oil	17.01	—
Pine silvestris oil	17.03	—
Dwarf pine oil	17.61	—
Frankincense oil	19.00	—
Juniper berry oil	20.58	—
Spruce needle oil	25.48	—
Cypress oil	25.91	—
Spearmint oil	27.34	—
Marjoram oil	29.85	—
Cumin oil	34.95	—
Silver fir oil	37.96	—
Ginger oil	40.86	—
Citrus oil	42.82	—
Hyssop oil	47.03	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Angelica root oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Angelica root oil	33019-109871BAG90451	30964	40	not required
Taoasis	Angelica root oil	4053-116078	31682	60	not required
Taoasis	Angelica root oil	2829199-122587	31780	60	not required
Taoasis	Angelica root oil	3029209-123992	32068	60	not required
Taoasis	Angelica root oil	B3039-9598	35074	40	not required
Taoasis	Angelica root oil	19515	38775	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 6 reference samples from the substance/substance group *Angelica root oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 6 different batches.
- 27 634 spectra from a total of 594 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Angelica root oil	3029209-125059	32477	40
Taoasis	Angelica root oil	1839219-127663	33644	40
Taoasis	Angelica root oil	17019-B-DE-R03	37651	40

- 30 810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 9 spectra from 5 *Apo-Ident* customers from 8 batches from the substance/substance group *Angelica root oil*.
- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Angelica root oil	11352706	1
Taoasis	Angelica root oil	1049239-3525	2
Taoasis	Angelica root oil	129271	1
Taoasis	Angelica root oil	294-926-9-13744	1
Taoasis	Angelica root oil	32229229-1384	1
Taoasis	Angelica root oil	33019-110236BAG904	1
Taoasis	Angelica root oil	3629209-126289	1
Taoasis	Angelica root oil	4053-117762	1

- 20 769 spectra from 1559 *Apo-Ident* customers from a total of 6344 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	300	0	27 634
Type B	0	120	0	30 810
Type C	0	9	0	20 769

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9615 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0638 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30964	30964	0.00	28.75
31682	31682	0.00	26.52
31780	31780	0.00	30.72
32068	32068	0.00	26.28
35074	35074	0.00	18.70
38775	38775	0.00	11.73

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Anise oil, organic**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30670-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Anise oil, organic

Special notes

When selecting the *Anise oil, organic* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Anise oil, organic	2	4	41

Second-stage model

For differentiation of the substance/substance group *Anise oil, organic* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Anise oil, organic* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Fennel oil	43.07	—
Basil oil	82.57	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Anise oil, organic*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Anise oil, organic	2241027-120475	31681	60	not required
Taoasis	Anise oil, organic	1492-125379	32794	40	not required
Taoasis	Anise oil, organic	1492-125379	32935	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 3 reference samples from the substance/substance group *Anise oil, organic*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 2 different batches.
- 27 794 spectra from a total of 598 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by

this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 200 spectra of 5 reference samples from the substance/substance group *Anise oil, organic*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Anise oil, organic	B080009-99431BAG90451	30670	40
Taoasis	Anise oil, organic	42803-290	33622	40
Taoasis	Anise oil, organic	42803-3438	34288	40
Taoasis	Anise oil, organic	11501-17140	37655	40
Taoasis	Anise oil, organic	42803-290	33875	40

- 30 730 spectra from a total of 705 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 55 spectra from 27 *Apo-Ident* customers from 43 batches from the substance/substance group *Anise oil, organic*.
- Among them are spectra of independent samples from 41 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Anise oil, organic	11501-17140	1
	Anise oil, organic	9502-16625C	1
Apotheker S Bauer&Comp	Anise oil, organic		1
Caelo	Anise oil, organic	12322503	1
Caelo	Anise oil, organic	12322507	1
Caelo	Anise oil, organic	13056105	1
Caelo	Anise oil, organic	15148901	1
Caelo	Anise oil, organic	17150001	1
Caelo	Anise oil, organic	182445002	1
Caelo	Anise oil, organic	183075006	1
Caelo	Anise oil, organic	18307510	1
Caelo	Anise oil, organic	18307513	4

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Supplier	Substance	Batch	Spectra
Caelo	Anise oil, organic	20003664001	2
Caelo	Anise oil, organic	20003664003	1
Phönix 10.04.2017	Anise oil, organic	15337020	1
primavera	Anise oil, organic	169k27	1
Schubert	Anise oil, organic	1236E0-1518	1
Taoasis GmbH	Anise oil, organic	2721-8434	1
Taoasis GmbH	Anise oil, organic	2721-8650	1
Taoasis GmbH	Anise oil, organic	6142-10446	1
Taoasis	Anise oil, organic	130910-113040	1
Taoasis	Anise oil, organic	1492-121627	1
Taoasis	Anise oil, organic	1492-123225	1
Taoasis	Anise oil, organic	1492-125315	1
Taoasis	Anise oil, organic	1492-125379	2
Taoasis	Anise oil, organic	2241027-120196	1
Taoasis	Anise oil, organic	2336-5388	1
Taoasis	Anise oil, organic	2336-7107	1
Taoasis	Anise oil, organic	2336-7299	1
Taoasis	Anise oil, organic	26569-115911	2
Taoasis	Anise oil, organic	26735-108555	1
Taoasis	Anise oil, organic	26735-110455	1
Taoasis	Anise oil, organic	26735-111137	2
Taoasis	Anise oil, organic	26735-113054	1
Taoasis	Anise oil, organic	2721-8434	1
Taoasis	Anise oil, organic	2721-8650	2
Taoasis	Anise oil, organic	42803-1177	1
Taoasis	Anise oil, organic	42803-127333	1
Taoasis	Anise oil, organic	42803-290	1
Taoasis	Anise oil, organic	42803-772	1
Taoasis	Anise oil, organic	8731-12846	1
Taoasis/Noweda	Anise oil, organic	1465-121083h08	1
Taoasis/Noweda	Anise oil, organic	2241027-120928H07	1
Taoasis/Sanacorp	Anise oil, organic	26735-111137	2
Taoasis/Sanacorp	Anise oil, organic	26735-112250	1
Taoasis/Taoasis	Anise oil, organic	9502-16625B	1

- 20 723 spectra from 1557 *Apo-Ident* customers from a total of 6309 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	140	0	27 794
Type B	0	175	25	30 690
Type C	0	51	4	20 723

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9618 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9569 %)	87.5000 % (> 86.0000 %)
Type C	100.0000 % (> 99.0591 %)	92.7273 % (> 87.2727 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31681	31681	0.00	43.07
32794	32794	0.00	45.20
32935	32935	0.00	48.36

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Banana aroma**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31105-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Banana aroma; Banana flavour

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Banana aroma	3	5	20

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Banana aroma* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Nicotine	114.98	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Banana aroma*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Banana aroma	12302509	31105	40	1404166
Caelo	Banana aroma	14353702	31606	60	not required
Caelo	Banana aroma	171890	33687	40	20170707*

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 3 reference samples from the substance/substance group *Banana aroma*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.

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

- 27 794 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 224 spectra of 6 reference samples from the substance/substance group *Banana aroma*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Banana aroma	16089305	33496	40
Caelo	Banana aroma	20004505002	36050	40
Caelo	Banana aroma	22001475003	36738	40
Caelo	Banana aroma	23002593	38414	40
Caelo	Banana aroma	25000505	39154	24
Caelo	Banana aroma	16089305	33608	40

- 30 706 spectra from a total of 704 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 63 spectra from 43 *Apo-Ident* customers from 21 batches from the substance/substance group *Banana aroma*.
- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Banana aroma	22001475001	2
	Banana aroma	22001475003	1
	Banana aroma	22001475004	1
	Banana aroma	22001475005	1
	Banana aroma	22001475006	1
	Banana aroma	23002593001	5
Caelo	Banana aroma	12302509	1

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Supplier	Substance	Batch	Spectra
Caelo	Banana aroma	14353707	1
Caelo	Banana aroma	14353709	1
Caelo	Banana aroma	16089304	2
Caelo	Banana aroma	16089305	2
Caelo	Banana aroma	17189001	5
Caelo	Banana aroma	17189002	3
Caelo	Banana aroma	18017201	2
Caelo	Banana aroma	18017202	1
Caelo	Banana aroma	18017205	2
Caelo	Banana aroma	191853001	4
Caelo	Banana aroma	19185301	4
Caelo	Banana aroma	2000450500	1
Caelo	Banana aroma	20004505001	5
Caelo	Banana aroma	20004505002	2
Caelo	Banana aroma	22001475003	2
Caesar & Loretz GmbH	Banana aroma	18017202	1
Caesar & Loretz GmbH	Banana aroma	18017205	1
Caesar & Loretz GmbH	Banana aroma	191853001	2
Caesar & Loretz GmbH	Banana aroma	20004505001	1
Caesar & Loretz GmbH	Banana aroma	20004505002	1
Caesar & Loretz GmbH	Banana aroma	22001475001	1
Caesar & Loretz GmbH	Banana aroma	22001475003	1
Caesar & Loretz GmbH	Banana aroma	22001475004	1
Caesar & Loretz GmbH	Banana aroma	22001475005	2
Caesar & Loretz GmbH...	Banana aroma	19185301	1
Phoenix	Banana aroma	20004505002	1
Sanacorp	Banana aroma	22001475003	1

- 20 715 spectra from 1559 *Apo-Ident* customers from a total of 6331 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	140	0	27 794
Type B	0	224	0	30 706
Type C	0	63	0	20 715

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9618 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 97.3214 %)
Type C	100.0000 % (> 99.0590 %)	100.0000 % (> 90.4762 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31105	31105	0.00	140.56
31606	31606	0.00	135.36
33687	33687	0.00	135.89

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Basil oil/Coriander oil/Thyme oil, white**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31552-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Basil oil/Coriander oil/Thyme oil, white; Basil oil; Coriander oil; Oleum coriandri; Oleum ocimum basilicum; Thyme oil, white

Special notes

When selecting the *Basil oil/Coriander oil/Thyme oil, white* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Basil oil/Coriander oil/Thyme oil, white	12	8	23

Second-stage model

For differentiation of the substance/substance group *Basil oil/Coriander oil/Thyme oil, white* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Basil oil/Coriander oil/Thyme oil, white* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Matricaria oil, morrocan	17.65	—
Neroli oil	27.80	—
Rosewood oil	47.49	—
Carrot seed oil	51.62	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Basil oil/Coriander oil/Thyme oil, white*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Basil oil	561-119057	31755	60	not required
Taoasis	Basil oil	1500312-128851	33725	40	not required
Taoasis	Basil oil	9272-17230	37656	40	not required
Taoasis	Coriander oil	9324-114961	31552	60	not required
Taoasis	Coriander oil	25134-117444	31690	60	not required
Taoasis	Coriander oil	104709-126301	32792	40	not required
Taoasis	Coriander oil	109291-2941	34286	40	not required
Primavera	Thyme oil, white	01067J25	33796	40	not required
Primavera	Thyme oil, white	00593E26	34176	40	not required
Primavera	Thyme oil, white	00470E31	37787	40	not required
Taoasis	Thyme oil, white	111400-970	33818	40	not required
Taoasis	Thyme oil, white	111806-16589	37673	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 540 spectra of 12 reference samples from the substance/substance group *Basil oil/Coriander oil/Thyme oil, white*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 12 different batches.
- 27 394 spectra from a total of 588 batches from further 141 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 360 spectra of 9 reference samples from the substance/substance group *Basil oil/Coriander oil/Thyme oil, white*.
- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Basil oil	21022-108746BAG90451	30751	40
Taoasis	Basil oil	1500312-126393	32972	40
Taoasis	Coriander oil	104709-127188	33053	40
Taoasis	Coriander oil	9291-1307	33990	40
Taoasis	Coriander oil	115804-16591	37684	40
Primavera	Thyme oil, white	00146J26	34293	40
Primavera	Thyme oil, white	00535M26	34369	40
Taoasis	Thyme oil, white	925	33819	40
Taoasis	Basil oil	1500312-126393	32973	40

- 30 570 spectra from a total of 701 batches from further 208 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 24 spectra from 19 *Apo-Ident* customers from 23 batches from the substance/substance group *Basil oil/Coriander oil/Thyme oil, white*.
- Among them are spectra of independent samples from 23 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Coriander oil	283-880-0	1
Apotheker Bauer & Ci...	Coriander oil	8008-52-4	1
Caelo	Coriander oil	15229607	1
Caelo	Coriander oil	16140401	1
Caelo	Coriander oil	16140410	1
Caelo	Coriander oil	17050408	1
Caelo	Coriander oil	19081002	1
Caesar & Loretz GmbH	Coriander oil	19081003	1
GEHE	Coriander oil	17050403	1
Gehe/Primavera	Thyme oil, white	340L29	1
Melasan	Coriander oil	1725704	1
Primavera, Gehe	Thyme oil, white	334A28	1
Primavera, Gehe	Thyme oil, white	78H27	1
primavera	Thyme oil, white	334A2B	1
Primavera	Thyme oil, white	340L29	1
Primavera	Thyme oil, white	442K31	1
Sanacorp	Coriander oil	18125703	1
Taoasis GmbH	Thyme oil, white	114133-9219	1
taoasis	Coriander oil	104709127	1
Taoasis	Thyme oil, white	112249-14868	1
Taoasis	Basil oil	6362-10840	1
Taoasis	Thyme oil, white	6512-13201	1
Taoasis	Thyme oil, white	6512-14244	1
Taoasis	Coriander oil	9291-1307	1

- 20 754 spectra from 1558 *Apo-Ident* customers from a total of 6329 batches from a further 164 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	540	0	27 394
Type B	0	359	1	30 570
Type C	0	23	1	20 754

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9614 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9564 %)	99.7222 % (> 98.8889 %)
Type C	100.0000 % (> 99.0603 %)	95.8333 % (> 83.3333 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31552	31552	0.00	54.19
31690	31690	0.00	66.11
31755	31755	0.00	166.47
32792	32792	0.00	59.53
33725	33725	0.00	190.28
33796	33796	0.00	29.42
33818	33818	0.00	58.90
34176	34176	0.00	31.31
34286	34286	0.00	53.97
37656	37656	0.00	69.26
37673	37673	0.00	63.66
37787	37787	0.00	36.96

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Benzoin siam oil 20%**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30456-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Benzoin siam oil 20%; Oleum styrax tonkinensis

Special notes

When selecting the *Benzoin siam oil 20%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Benzoin siam oil 20%	6	2	15

Second-stage model

For differentiation of the substance/substance group *Benzoin siam oil 20%* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Benzoin siam oil 20%* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Siam benzoin (solution)	72.53	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Benzoin siam oil 20%* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Benzoin siam oil 20%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Benzoin siam oil 20%	12990-114892	31256	40	not required
Taoasis	Benzoin siam oil 20%	51939-123084	31843	60	not required
Taoasis	Benzoin siam oil 20%	63287-126233	32974	40	not required
Taoasis	Benzoin siam oil 20%	2161-1395	33855	40	not required
Taoasis	Benzoin siam oil 20%	32105-119788BAG90451	33944	40	not required
Taoasis	Benzoin siam oil 20%	17293-LA-R05	37653	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Benzoin siam oil 20%*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 6 different batches.
- 27 674 spectra from a total of 594 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this

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

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

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

- 120 spectra of 3 reference samples from the substance/substance group *Benzoin siam oil 20%*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Benzoin siam oil 20%	2010-836	33724	40
Taoasis	Benzoin siam oil 20%	20278	38779	40
Taoasis	Benzoin siam oil 20%	63287-126233	33028	40

- 30810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 18 spectra from 8 *Apo-Ident* customers from 17 batches from the substance/substance group *Benzoin siam oil 20%*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis	Benzoin siam oil 20%	17578-116819	1
Taoasis	Benzoin siam oil 20%	23478-116955	2
Taoasis	Benzoin siam oil 20%	31343-118365	1
Taoasis	Benzoin siam oil 20%	41242-120661	1
Taoasis	Benzoin siam oil 20%	41242-121512	1
Taoasis	Benzoin siam oil 20%	518434-108321	1
Taoasis	Benzoin siam oil 20%	51939-123084	1
Taoasis	Benzoin siam oil 20%	54125	1
Taoasis	Benzoin siam oil 20%	541389-111081	1
Taoasis	Benzoin siam oil 20%	548442-113119	1
Taoasis	Benzoin siam oil 20%	548481-111780	1
Taoasis	Benzoin siam oil 20%	59023-125420	1

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Supplier	Substance	Batch	Spectra
Taoasis	Benzoin siam oil 20%	62330-124547	1
Taoasis	Benzoin siam oil 20%	63287-126233	1
Taoasis	Benzoin siam oil 20%	8071-12402	1
Taoasis	Benzoin siam oil 20%	8211-13793	1
Taoasis	Benzoin siam oil 20%	474084-96350	1

- 20 760 spectra from 1559 *Apo-Ident* customers from a total of 6335 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Benzoin siam oil 20%* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Benzoin siam oil 20%* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	27 674
Type B	0	119	1	30 810
Type C	0	17	1	20 760

The substance/substance group *Benzoin siam oil 20%* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9566 %)	99.1667 % (> 96.6667 %)
Type C	100.0000 % (> 99.0610 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31256	31256	0.00	93.66
31843	31843	0.00	93.35
32974	32974	0.00	98.60
33855	33855	0.00	99.73
33944	33944	0.00	102.77
37653	37653	0.00	95.49

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Bergamot oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30307-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Bergamot oil; Oleum citrus bergamia

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Bergamot oil	5	2	26

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bergamot oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Chamomile (essential oil)	31.05	—
Spearmint oil	32.11	—
Grapefruit oil, organic	43.06	—
Myrrh oil	44.65	—
Dwarf pine oil	51.00	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Bergamot oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Bombastus	Bergamot oil	290998	31641	60	not required
Bombastus	Bergamot oil	290998	31760	60	not required
Bombastus	Bergamot oil	23000284	36887	40	not required
Primavera	Bergamot oil	00111A32	37972	40	not required
Taoasis	Bergamot oil	3221028-121642	31784	60	not required
Taoasis	Bergamot oil	01/22BE-16535	37657	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 6 reference samples from the substance/substance group *Bergamot oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5

different batches.

- 27 634 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Bergamot oil	00189A27	34387	40
Taoasis	Bergamot oil	1968-128263	33437	40

- 30 850 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 28 spectra from 24 *Apo-Ident* customers from 26 batches from the substance/substance group *Bergamot oil*.
- Among them are spectra of independent samples from 26 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Bergamot oil	21000945017	1
Bombastus	Bergamot oil	19006566	2
Bombastus	Bergamot oil	20002503	1
Bombastus	Bergamot oil	21004665	1
Bombastus	Bergamot oil	264008	1
Bombastus	Bergamot oil	280260	1
Bombastus	Bergamot oil	53731-125890	1
Caelo	Bergamot oil	12020702	1
Caelo	Bergamot oil	13141501	2

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Supplier	Substance	Batch	Spectra
Caelo	Bergamot oil	192330002	1
Caelo	Bergamot oil	192330009	1
Caelo	Bergamot oil	21000945006	1
Caelo	Bergamot oil	21000945016	1
Caelo	Bergamot oil	7962	1
Kaders	Bergamot oil	130564	1
Noweda	Bergamot oil	271858	1
Primavera/Phoenix	Bergamot oil	30K30	1
Taoasis	Bergamot oil	32338-109135	1
Taoasis	Bergamot oil	32579-111866	1
Taoasis	Bergamot oil	33697-112408	1
Taoasis	Bergamot oil	6267IT-L02	1
Taoasis	Bergamot oil	73340-506	1
Taoasis	Bergamot oil	77879-3984	1
Taoasis	Bergamot oil	96243	1
Taoasis	Bergamot oil	B130301-110610	1
Taoasis	Bergamot oil	d01be14m-121110bag90	1

- 20 750 spectra from 1558 *Apo-Ident* customers from a total of 6326 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	300	0	27 634
Type B	0	80	0	30 850
Type C	0	28	0	20 750

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9615 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0600 %)	100.0000 % (> 78.5714 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31641	31641	0.00	35.93
31760	31760	0.00	33.77
31784	31784	0.00	32.37
36887	36887	0.00	42.10
37657	37657	0.00	53.97
37972	37972	0.00	46.84

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group	Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil
Substance class	BR APIs & excipients, liquid/semi-solid (other)
Report date	28/04/2026
Report number	30966-2026-04-28
Executing company	HiperScan GmbH Gerokstraße 13 01307 Dresden Germany

Relevant substance names

Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil; Cajeput (essentiel oil); Eucalyptus oil; Niaouli oil; Oleum Cajeputi artificiale; Oleum eucalypti; Oleum niaouli; Oleum rosmarini; Rosemary oil

Special notes

When selecting the *Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	<i>European Pharmacopoeia 11th Edition, Basic Version 2022</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA010	<i>Creation of IdentModule Updates</i>

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil	20	10	156

Second-stage model

For differentiation of the substance/substance group *Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Rosemary camphor oil	11.65	—
Immortelle oil	19.72	—
Cypress oil	23.27	—
Myrtle oil	23.75	—
Citus oil	25.64	—
Ravintsara oil	29.13	—
Hyssop oil	30.23	—
Sage oil	31.21	—
Marjoram oil	36.60	—
Vetiver bourbon oil	37.49	—
Angelica root oil	42.85	—
Spruce needle oil	44.00	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Cajeput (essentiel oil)	00012A27	34401	40	not required
Taoasis	Cajeput (essentiel oil)	130829-112094BAG90451	31136	40	not required
Taoasis	Cajeput (essentiel oil)	1662-124326	32173	40	not required
Taoasis	Cajeput (essentiel oil)	1724-127033	33657	40	not required
Taoasis	Cajeput (essentiel oil)	H007113-16953	37658	40	not required
Primavera	Eucalyptus oil	00178A27	34374	40	not required
Primavera	Eucalyptus oil	00500J31	37788	40	not required
Taoasis	Eucalyptus oil	527885-109705A	30966	40	not required
Taoasis	Eucalyptus oil	7271001-121014	31694	60	not required
Taoasis	Eucalyptus oil	043127A-125381	32903	40	not required

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Eucalyptus oil	10991-16557	37661	40	not required
Caelo	Niaouli oil	13099606	31420	60	AR-14-FG-012561-01
Primavera	Niaouli oil	00410K26	34380	40	not required
Taoasis	Niaouli oil	34167-116962	31548	60	not required
Taoasis	Niaouli oil	40428-124242	32174	40	not required
Taoasis	Niaouli oil	1500450-125771	32970	40	not required
Taoasis	Rosemary oil	3231031-117639	31551	60	not required
Taoasis	Rosemary oil	1921019-120666	31691	60	not required
Taoasis	Rosemary oil	1862-126630	32933	40	not required
Taoasis	Rosemary oil	2150-2819	34104	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 900 spectra of 20 reference samples from the substance/substance group *Cajeput oil / Eucalyptus oil / Niaouli oil / Rosemary oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 20 different batches.
- 27 034 spectra from a total of 580 batches from further 140 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 520 spectra of 13 reference samples from the substance/substance group *Cajeput oil / Eucalyptus oil / Niaouli oil / Rosemary oil*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Cajeput (essentiell oil)	2216-2921	34114	40
Primavera	Eucalyptus oil	00650K25	33808	40
Primavera	Eucalyptus oil	00256A26	33955	40
Primavera	Eucalyptus oil	00710C26	34172	40
Primavera	Eucalyptus oil	00190J31	37780	40
Taoasis	Eucalyptus oil	41192-129138	33621	40
Taoasis	Niaouli oil	1500450-1985	34040	40
Taoasis	Niaouli oil	8534-16209	37688	40

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Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Rosemary oil	1614-125089	32802	40
Taoasis	Rosemary oil	B022921-16229	37671	40
Taoasis	Cajeput (essentiel oil)	1724-127033	33022	40
Taoasis	Cajeput (essentiel oil)	1724-127033	33023	40
Taoasis	Niaouli oil	1500450-125771	32971	40

- 30 410 spectra from a total of 697 batches from further 207 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 219 spectra from 104 *Apo-Ident* customers from 160 batches from the substance/substance group *Cajeput oil* / *Eucalyptus oil* / *Niaouli oil* / *Rosemary oil*.
- Among them are spectra of independent samples from 156 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Rosemary oil	17953TNR08	1
	Niaouli oil	19003MGS04	1
	Rosemary oil	22000012005	1
	Rosemary oil	22000012016	1
	Rosemary oil	22000012022	1
	Eucalyptus oil	22002648004	1
	Rosemary oil	22005135	1
	Eucalyptus oil	23001429007	1
	Rosemary oil	23002482005	1
	Rosemary oil	23004465	1
	Rosemary oil	24004409	1
	Rosemary oil	24J00115	1
	Rosemary oil	25001901	1
	Niaouli oil	8534-16209	1
	Cajeput (essentiel oil)	H007113-16953	1
AHD	Rosemary oil	23004606	1
Apothker Bauer & Cie. oHG	Rosemary oil		1
ASAV	Eucalyptus oil	283-406-2	1
Aurica	Cajeput (essentiel oil)	11024710	1
Bauer	Niaouli oil	6558611608	1
Bergland	Eucalyptus oil	K801202	2
Bombastus	Cajeput (essentiel oil)	18001011	1
Bombastus	Eucalyptus oil	18005784	1
Bombastus	Eucalyptus oil	18006426	1
Bombastus	Eucalyptus oil	19002892	1
Bombastus	Eucalyptus oil	19004174	1
Bombastus	Eucalyptus oil	19005837	1
Bombastus	Rosemary oil	21000910	1
Bombastus	Eucalyptus oil	21001239	2
Bombastus	Eucalyptus oil	21003689	1
Bombastus	Cajeput (essentiel oil)	22005053	2
Bombastus	Eucalyptus oil	289701	1
Bombastus	Eucalyptus oil	297737	1

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Supplier	Substance	Batch	Spectra
Bombastus	Rosemary oil	301449	2
Bombastus	Eucalyptus oil	303327	2
Bombastus	Eucalyptus oil	303336	1
Bombastus	Eucalyptus oil	305608	1
Bombastus	Eucalyptus oil	305628	1
Bombastus	Cajeput (essentiel oil)	307412	1
Bombastus	Eucalyptus oil	307667	1
Bombastus	Eucalyptus oil	89(307667)	1
Caelo	Eucalyptus oil	11324112	1
Caelo	Eucalyptus oil	13106407LOT	1
Caelo	Eucalyptus oil	14039603	1
Caelo	Eucalyptus oil	15063309	1
Caelo	Eucalyptus oil	15400202	3
Caelo	Eucalyptus oil	15400203	2
Caelo	Eucalyptus oil	15400206	1
Caelo	Eucalyptus oil	15400217	1
Caelo	Rosemary oil	15442017	2
Caelo	Rosemary oil	16276903	1
Caelo	Rosemary oil	16276905	1
Caelo	Niaouli oil	16312603	1
Caelo	Eucalyptus oil	16351301	1
Caelo	Eucalyptus oil	16351309	1
Caelo	Eucalyptus oil	16351312	3
Caelo	Eucalyptus oil	16351313	1
Caelo	Eucalyptus oil	1703030-01	1
Caelo	Rosemary oil	17326714	1
Caelo	Eucalyptus oil	17337701	1
Caelo	Eucalyptus oil	18171701	2
Caelo	Eucalyptus oil	18171714	1
Caelo	Eucalyptus oil	19016712	1
Caelo	Rosemary oil	191803011	5
Caelo	Eucalyptus oil	192938006	1
Caelo	Rosemary oil	200009011	1
Caelo	Rosemary oil	20004109011	3
Caelo	Rosemary oil	20004109013	1
Caelo	Eucalyptus oil	20004134004	1
Caelo	Rosemary oil	200042109012	1
Caelo	Eucalyptus oil	20004332010	1
Caelo	Rosemary oil	22000012001	1
Caelo	Rosemary oil	22000012005	1
Caelo	Rosemary oil	22000012013	1
Caelo	Eucalyptus oil	300881	1
Caelo	Rosemary oil	306506	1
Caelo	Rosemary oil	55(16276903)	1
Caesar & Loretz GmbH...	Eucalyptus oil	15063312	1
Caesar & Loretz GmbH...	Eucalyptus oil	15400203	1
Eurho/Sanacorp	Rosemary oil	2205009-01	1
Euro OTC	Eucalyptus oil	1412030-01	1
Euro OTC	Rosemary oil	151101602	1
Euro OTC	Eucalyptus oil	22003155	1
Kögl	Eucalyptus oil	397311160117	1
Noweda	Cajeput (essentiel oil)	7204349	1
Noweda	Eucalyptus oil	8819ES-Mo1	1
Phönix	Eucalyptus oil	23000071	1
Primavera	Niaouli oil	410K26	1
Primavera	Cajeput (essentiel oil)	424A28	1
PVL	Cajeput (essentiel oil)	150712	1
Sanacorp	Cajeput (essentiel oil)	22005053	1
TAOASIS GmbH D-32758...	Cajeput (essentiel oil)	1989-2818	1
Taoasis	Eucalyptus oil	107371-6271	2

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Supplier	Substance	Batch	Spectra
Taoasis	Niaouli oil	108478-13745	1
Taoasis	Cajeput (essentiel oil)	1301-121889	1
Taoasis	Cajeput (essentiel oil)	1301-32758	1
Taoasis	Eucalyptus oil	130205-111868	1
Taoasis	Cajeput (essentiel oil)	130829-113045	1
Taoasis	Cajeput (essentiel oil)	131010-115487	2
Taoasis	Cajeput (essentiel oil)	131010-117241	2
Taoasis	Cajeput (essentiel oil)	131010-117257	1
Taoasis	Niaouli oil	1500450-125771	1
Taoasis	Niaouli oil	1500450-12690	1
Taoasis	Niaouli oil	1500450-9867	1
Taoasis	Cajeput (essentiel oil)	1518-122691	1
Taoasis	Cajeput (essentiel oil)	1518-122790	1
Taoasis	Rosemary oil	1526-123355	1
Taoasis	Rosemary oil	1526-125088	1
Taoasis	Eucalyptus oil	156805-12300	1
Taoasis	Eucalyptus oil	156805-12301	1
Taoasis	Rosemary oil	1614-125089	12
Taoasis	Cajeput (essentiel oil)	1662-124870	1
Taoasis	Cajeput (essentiel oil)	1724-125910	1
Taoasis	Cajeput (essentiel oil)	1724-126425	1
Taoasis	Cajeput (essentiel oil)	1724-127010	2
Taoasis	Cajeput (essentiel oil)	1724-127033	1
Taoasis	Cajeput (essentiel oil)	1724-127654	1
Taoasis	Cajeput (essentiel oil)	1724-129091	1
Taoasis	Rosemary oil	1862-127716	1
Taoasis	Rosemary oil	1862-128861	1
Taoasis	Cajeput (essentiel oil)	1967	1
Taoasis	Rosemary oil	1972-2523	2
Taoasis	Rosemary oil	1972-773	2
Taoasis	Cajeput (essentiel oil)	1989-1032	2
Taoasis	Cajeput (essentiel oil)	1989-955	3
Taoasis	Cajeput (essentiel oil)	1989-956	1
Taoasis	Niaouli oil	22553-120413	1
Taoasis	Niaouli oil	22553-120482	1
Taoasis	Niaouli oil	22553-121510	1
Taoasis	Rosemary oil	2331-2821	2
Taoasis	Rosemary oil	2331-6428	1
Taoasis	Cajeput (essentiel oil)	24077-106468	1
Taoasis	Cajeput (essentiel oil)	2490-4102	3
Taoasis	Cajeput (essentiel oil)	2490-5372	2
Taoasis	Cajeput (essentiel oil)	2490-6100	2
Taoasis	Rosemary oil	26057-119164	1
Taoasis	Rosemary oil	26057-122996	1
Taoasis	Eucalyptus oil	33364-110871	1
Taoasis	Niaouli oil	40428-123092	1
Taoasis	Niaouli oil	40428-128260	4
Taoasis	Eucalyptus oil	43703-122178	1
Taoasis	Eucalyptus oil	43703-122404	1
Taoasis	Eucalyptus oil	52046-124692	2
Taoasis	Eucalyptus oil	543495-112704	1
Taoasis	Cajeput (essentiel oil)	661027-117257	2
Taoasis	Cajeput (essentiel oil)	661027-118368	1
Taoasis	Eucalyptus oil	67253-127038	2
Taoasis	Cajeput (essentiel oil)	6781012-119058	1
Taoasis	Eucalyptus oil	75793-129093	2
Taoasis	Eucalyptus oil	79948-858	1
Taoasis	Eucalyptus oil	82675-1874	1
Taoasis	Eucalyptus oil	91092-3355	2
Taoasis	Eucalyptus oil	98837-4013	1

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Supplier	Substance	Batch	Spectra
Taoasis	Eucalyptus oil	98937-4013	1
Taoasis	Eucalyptus oil	98937-5299	2
Taoasis	Cajeput (essentiel oil)	AR1906451-10605	4
Taoasis	Cajeput (essentiel oil)	AR1906451-10606	1
Taoasis	Cajeput (essentiel oil)	H007113-14497	1
Taoasis	Cajeput (essentiel oil)	L201323018-113057	1
Taoasis/Noweda	Niaouli oil	5091MGK10	1
Taoasis/Sanacorp	Cajeput (essentiel oil)	AR1906451x2	1
Taoasis/Sanacorp	Cajeput (essentiel oil)	L201323018-113057	1
Taoasis/Taoasis	Rosemary oil	128391-ESJ05	1
Taoasis/Taoasis	Niaouli oil	1500450-5752	1

- 20 559 spectra from 1558 *Apo-Ident* customers from a total of 6192 batches from a further 163 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	900	0	27 034
Type B	0	520	0	30 410
Type C	0	215	4	20 559

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9613 %)	100.0000 % (> 99.3333 %)
Type B	100.0000 % (> 99.9564 %)	100.0000 % (> 98.8462 %)
Type C	100.0000 % (> 99.0584 %)	98.1735 % (> 96.8037 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30966	30966	0.00	45.71
31136	31136	0.00	59.46
31420	31420	0.00	29.31
31548	31548	0.00	52.06
31551	31551	0.00	24.68
31691	31691	0.00	18.81
31694	31694	0.00	43.53
32173	32173	0.00	57.18
32174	32174	0.00	42.36
32903	32903	0.00	32.23
32933	32933	0.00	30.79
32970	32970	0.00	48.06
33657	33657	0.00	59.08
34104	34104	0.00	26.23
34374	34374	0.00	38.63
34380	34380	0.00	47.15
34401	34401	0.00	64.47
37658	37658	0.00	56.57
37661	37661	0.00	30.22
37788	37788	0.00	59.21

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Camphor oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 33826-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Camphor oil

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Camphor oil	3	1	0

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Camphor oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Angelica root oil	15.20	—
Marjoram oil	25.16	—
Hyssop oil	26.50	—
Silver fir oil	27.20	—
Cumin oil	33.33	—
Frankincense oil	35.10	—
Citus oil	35.97	—
Sage oil	40.49	—
Myrtle oil	40.51	—
Swiss pine oil	41.15	—
Spruce needle oil	42.87	—
Cypress oil	43.21	—
Rosemary oil	45.72	—
Ravintsara oil	51.76	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Camphor oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Camphor oil	74521-140	33826	40	not required
Taoasis	Camphor oil	944	33827	40	not required
Taoasis	Camphor oil	18318	38781	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Camphor oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.
- 27 814 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Camphor oil	78793-2563	34039	40

- 30 890 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Camphor oil*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 20 778 spectra from 1559 *Apo-Ident* customers from a total of 6352 batches from a further 167 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#),

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

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	120	0	27 814
Type B	0	40	0	30 890
Type C	0	0	0	20 778

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9619 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9570 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.0752 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33826	33826	0.00	30.83
33827	33827	0.00	30.36
38781	38781	0.00	26.05

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Cardamom oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 33813-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Cardamom oil; Cardamom (essential oil)

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Cardamom oil	2	1	4

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cardamom oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citrus oil	28.40	—
Vetiver bourbon oil	32.09	—
Matricaria oil, roman	34.74	—
Manuka oil	35.14	—
Myrtle oil	43.42	—
Sage oil	45.16	—
Hyssop oil	47.21	—
Cumin oil	50.80	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Cardamom oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Cardamom oil	00897G25	33813	40	not required
Primavera	Cardamom oil	00080M25	33961	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Cardamom oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 2 different batches.

- 27 854 spectra from a total of 598 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Cardamom oil	00498H26	34291	40

- 30 890 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 5 spectra from 2 *Apo-Ident* customers from 4 batches from the substance/substance group *Cardamom oil*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Bahnhof-Apotheke	Cardamom oil	AP200925-01	1
Primavera	Cardamom oil	291F28	1
Taoasis	Cardamom oil	12207C0-N03	1
Taoasis	Cardamom oil	13749C0-N09	2

- 20 773 spectra from 1559 *Apo-Ident* customers from a total of 6348 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	80	0	27 854
Type B	0	40	0	30 890
Type C	0	5	0	20 773

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9623 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9570 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.0683 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33813	33813	0.00	39.78
33961	33961	0.00	39.72

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Carrot seed oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31555-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Carrot seed oil; Oleum daucus carota

Special notes

When selecting the *Carrot seed oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Carrot seed oil	4	2	3

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Carrot seed oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	21.28	—
Tea tree oil	23.61	—
Lemon grass oil	38.44	—
Matricaria oil, morrocan	38.75	—
Patchouli oil	41.20	—
Vetiver bourbon oil	42.69	—
Thyme oil, white	43.53	—
Ginger oil	44.26	—
Citrus oil	56.52	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Carrot seed oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Carrot seed oil	937-117443	31555	60	not required
Taoasis	Carrot seed oil	1775-125361BAG90451	32812	40	not required
Taoasis	Carrot seed oil	3496IN-K08	34282	40	not required
Taoasis	Carrot seed oil	19063	38600	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Carrot seed oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 754 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 140 spectra of 3 reference samples from the substance/substance group *Carrot seed oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Carrot seed oil	26058-119083BAG90451	31636	60
Taoasis	Carrot seed oil	2037	33995	40
Taoasis	Carrot seed oil	1775-125361BAG90451	33203	40

- 30 790 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 3 spectra from 1 *Apo-Ident* customers from 3 batches from the substance/substance group *Carrot seed oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis	Carrot seed oil		1
Taoasis	Carrot seed oil	12585IN-N06	1
Taoasis	Carrot seed oil	14275B-INN11	1

- 20 775 spectra from 1559 *Apo-Ident* customers from a total of 6349 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	180	0	27 754
Type B	0	140	0	30 790
Type C	0	3	0	20 775

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.0750 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31555	31555	0.00	40.52
32812	32812	0.00	53.75
34282	34282	0.00	49.86
38600	38600	0.00	53.96

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

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Cedar wood oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30654-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Cedar wood oil; Oleum cedrus deodara

Special notes

When selecting the *Cedar wood oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Cedar wood oil	3	4	21

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cedar wood oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Vetiver bourbon oil	17.76	—
Citrus oil	17.88	—
Hyssop oil	20.22	—
Immortelle oil	21.90	—
Marjoram oil	25.86	—
Myrtle oil	26.40	—
Ginger oil	26.65	—
Lemon grass oil	27.04	—
Cypress oil	29.74	—
Rosemary oil	34.82	—
Yarrow oil	35.41	—
Angelica root oil	39.81	—
Sage oil	43.41	—
Cajepout (essentielle oil)	43.64	—
Manuka oil	46.11	—
Matricaria oil, morrocan	47.02	—
Frankincense oil	49.43	—
Rosemary camphor oil	49.56	—
Niaouli oil	51.11	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Cedar wood oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Apotheker ...	Cedar wood oil	2.880926.1507	31851	60	not required
Taoasis	Cedar wood oil	7891018-121034	31777	60	not required
Taoasis	Cedar wood oil	1627-125061	33199	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 3 reference samples from the substance/substance group *Cedar wood oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.
- 27 774 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Cedar wood oil	26473-83914BAG90451	30750	40
Taoasis	Cedar wood oil	1627-124623	32268	40
Taoasis	Cedar wood oil	1802-1975	34102	40
Taoasis	Cedar wood oil	102184-17065	37676	40

- 30 770 spectra from a total of 705 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 31 spectra from 3 *Apo-Ident* customers from 22 batches from the substance/substance group *Cedar wood oil*.
- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Biofrid / Noweda	Cedar wood oil	17066	1
Taoasis	Cedar wood oil	1627-125061	2
Taoasis	Cedar wood oil	1627-125917	1
Taoasis	Cedar wood oil	1627-127827	1
Taoasis	Cedar wood oil	1802-128288	3
Taoasis	Cedar wood oil	1802-1975	1
Taoasis	Cedar wood oil	1802-750	3
Taoasis	Cedar wood oil	1802-972	1
Taoasis	Cedar wood oil	18302-128288	1
Taoasis	Cedar wood oil	2339-3450	1
Taoasis	Cedar wood oil	2339-3615	2
Taoasis	Cedar wood oil	32812-113008	3
Taoasis	Cedar wood oil	381008-116967	1
Taoasis	Cedar wood oil	461016-6429	1
Taoasis	Cedar wood oil	7711023-120348	1
Taoasis	Cedar wood oil	7891018-120108	1
Taoasis	Cedar wood oil	7891019-121034	1
Taoasis	Cedar wood oil	831018-122540	1
Taoasis	Cedar wood oil	831018-123089	2
Taoasis	Cedar wood oil	831018-124172	1
Taoasis	Cedar wood oil	SAP709-5143	1
Taoasis/Phönix	Cedar wood oil	3292687	1

- 20 747 spectra from 1559 *Apo-Ident* customers from a total of 6331 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	160	0	27 774
Type B	0	120	40	30 770
Type C	0	31	0	20 747

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9618 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9565 %)	75.0000 % (> 73.1250 %)
Type C	100.0000 % (> 99.0598 %)	100.0000 % (> 80.6452 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31777	31777	0.00	70.86
31851	31851	0.00	20.22
33199	33199	0.00	68.44

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Chamomile (essential oil)**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 33811-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Chamomile (essential oil)

Special notes

When selecting the *Chamomile (essential oil)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Chamomile (essential oil)	5	3	1

Second-stage model

For differentiation of the substance/substance group *Chamomile (essential oil)* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Chamomile (essential oil)* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Bergamot oil	12.64	—
Melissa oil	23.90	—
Spearmint oil	35.18	—
Lemon grass oil	40.89	—
Vetiver bourbon oil	41.33	—
Citronella oil	43.85	—
Carrot seed oil	43.85	—
Marjoram oil	45.19	—
Ginger oil	54.27	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Chamomile (essential oil)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Chamomile (essential oil)	00888G25	33811	40	not required
Primavera	Chamomile (essential oil)	00715L25	33963	40	not required
Primavera	Chamomile (essential oil)	00520L31	37973	40	not required
Taoasis	Chamomile (essential oil)	2132-1981	33952	40	not required
Taoasis	Chamomile (essential oil)	5412-17146	37683	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Chamomile (essential oil)*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27734 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Chamomile (essential oil)	00139C26	34167	40
Taoasis	Chamomile (essential oil)	100477-850	33824	40
Taoasis	Chamomile (essential oil)	934	33825	40

- 30810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Chamomile (essential oil)*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Primavera/Noweda	Chamomile (essential oil)	229H27	1
Taoasis/Taoasis	Chamomile (essential oil)	2132-1981	1

- 20 776 spectra from 1559 *Apo-Ident* customers from a total of 6350 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	97	23	30 810
Type C	0	2	0	20 776

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9566 %)	80.8333 % (> 78.3333 %)
Type C	100.0000 % (> 99.0834 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33811	33811	0.00	49.60
33952	33952	0.00	22.23
33963	33963	0.00	50.06
37683	37683	0.00	67.22
37973	37973	0.00	25.99

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

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Cinnamon bark oil, Ceylon**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30957-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Cinnamon bark oil, Ceylon; Oleum cinnamomi ceylanici

Special notes

When selecting the *Cinnamon bark oil, Ceylon* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Cinnamon bark oil, Ceylon	5	1	5

Second-stage model

For differentiation of the substance/substance group *Cinnamon bark oil, Ceylon* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cinnamon bark oil, Ceylon* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Siam benzoin (solution)	106.50	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Cinnamon bark oil, Ceylon*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Cinnamon bark oil, Ceylon	00221A27	34375	40	not required
Taoasis	Cinnamon bark oil, Ceylon	121108-109782BAG90451	30957	40	not required
Taoasis	Cinnamon bark oil, Ceylon	1311130547-119819	31648	60	not required
Taoasis	Cinnamon bark oil, Ceylon	415-770	34107	40	not required
Taoasis	Cinnamon bark oil, Ceylon	2021110399-17127	37796	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 5 reference samples from the substance/substance group *Cinnamon bark oil, Ceylon*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 714 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are

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

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

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

- 80 spectra of 2 reference samples from the substance/substance group *Cinnamon bark oil, Ceylon*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Cinnamon bark oil, Ceylon	415-126411	32791	40
Taoasis	Cinnamon bark oil, Ceylon	415-126411	33202	40

- 30850 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 8 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Cinnamon bark oil, Ceylon*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cinnamon bark oil, Ceylon	23003206002	1
jacoby	Cinnamon bark oil, Ceylon	24J01644	1
Taoasis	Cinnamon bark oil, Ceylon	12217IN-N02	1
Taoasis	Cinnamon bark oil, Ceylon	415-129078	4
Taoasis/Sanacorp/06...	Cinnamon bark oil, Ceylon	1787-10972	1

- 20770 spectra from 1558 *Apo-Ident* customers from a total of 6347 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	220	0	27 714
Type B	0	80	0	30 850
Type C	0	8	0	20 770

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0645 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30957	30957	0.00	219.38
31648	31648	0.00	180.69
34107	34107	0.00	182.70
34375	34375	0.00	106.50
37796	37796	0.00	210.69

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Citric oil / Lime oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31544-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Citric oil / Lime oil; Citric oil; Lime oil; Oleum citri; Oleum citrus aurantifolia

Special notes

When selecting the *Citric oil / Lime oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Citric oil / Lime oil	8	5	98

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citric oil* / *Lime oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mandarin oil, green	17.71	—
Grapefruit oil, organic	21.76	—
Dwarf pine oil	30.93	—
Silver fir oil	33.98	—
Orange oil	34.44	—
Tea tree oil	41.52	—
Marjoram oil	45.72	—
Cypress oil	53.11	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Citric oil* / *Lime oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Citric oil	D04LI14M-117513	31558	60	not required
Taoasis	Citric oil	3681027-122724	31838	60	not required
Taoasis	Citric oil	127939-ITJ04	33611	40	not required
Primavera	Lime oil	00182A27	34393	80	not required
Taoasis	Lime oil	059-117571	31544	60	not required
Taoasis	Lime oil	15506-1458	33874	40	not required
Taoasis	Lime oil	15506-1762	33942	40	not required
Taoasis	Lime oil	2021110901-14858	37664	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 420 spectra of 8 reference samples from the substance/substance group *Citric oil / Lime oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 8 different batches.
- 27 514 spectra from a total of 592 batches from further 142 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 340 spectra of 8 reference samples from the substance/substance group *Citric oil / Lime oil*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Citric oil	00011A27	34379	40
Taoasis	Citric oil	03LI16M-125453I09	32771	40
Taoasis	Citric oil	20142	38773	40
Taoasis	Lime oil	867-124956	32800	40
Taoasis	Lime oil	20285	38776	40
Taoasis	Citric oil	03LI16M-125453I09	32941	40
Taoasis	Lime oil	059-117571	31654	60
Taoasis	Lime oil	867-124956	32976	40

- 30 590 spectra from a total of 703 batches from further 209 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 144 spectra from 107 *Apo-Ident* customers from 101 batches from the substance/substance group *Citric oil / Lime oil*.
- Among them are spectra of independent samples from 97 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Citric oil		1
	Citric oil	147H30	1
	Citric oil	187K31	1
	Citric oil	188M31	1
	Citric oil	22001195015	1
	Citric oil	22004097006	2
	Citric oil	22004097011	2
	Citric oil	2300210265/23P	1
	Citric oil	23002829005	3
	Citric oil	24J01278	1
	Citric oil	463E31	1
Bergland	Citric oil		1
Bergland	Citric oil	K603901	1
bergland	Citric oil	K703167	1
Bergland	Citric oil	K902012	1
Bergland/Noweda	Citric oil	P111077	1
Bombastaus	Citric oil	21004056	1
Bombastus	Citric oil	12268005-1-0	1
Bombastus	Citric oil	15F29-B04-325354	1
Bombastus	Citric oil	18006427	1
Bombastus	Citric oil	19002045	1
Bombastus	Citric oil	19003199	1
Bombastus	Citric oil	19003228	3
Bombastus	Citric oil	20002625	1
Bombastus	Citric oil	20005153	1
Bombastus	Citric oil	21001992	1
Bombastus	Citric oil	22001026	1
Bombastus	Citric oil	260253	1
Bombastus	Citric oil	297506	1
Bombastus	Citric oil	301912	1
Bombastus	Citric oil	302311	1
Bombastus	Citric oil	304030	1
Caelo	Citric oil	14365212	3
Caelo	Citric oil	14385201	1
Caelo	Citric oil	15182703	3
Caelo	Citric oil	15182711	1
Caelo	Citric oil	16028702	3
Caelo	Citric oil	16028719	2
Caelo	Citric oil	16275202	2
Caelo	Citric oil	16275203	1
Caelo	Citric oil	16275206	1
Caelo	Citric oil	16275213	1
Caelo	Citric oil	16275216	5
Caelo	Citric oil	17106807	5
Caelo	Citric oil	17321101	1
Caelo	Citric oil	17321104	2
Caelo	Citric oil	18092202	4
Caelo	Citric oil	18092216	2
Caelo	Citric oil	18328003	4
Caelo	Citric oil	20004025013	1
Caelo	Citric oil	21003697003	1
Caelo	Citric oil	2200048005	1
Caelo	Citric oil	22001195001	1
Caelo	Citric oil	22001195005	1
Caelo	Citric oil	22001195008	1
Caelo	Citric oil	2416Q-01973	1
Caelo	Citric oil	91(18092216)	1
Caelo	Citric oil	W373	1
Caesar & Loretz GmbH	Citric oil	22004097008	1
Casida	Citric oil	CA3A	1

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Supplier	Substance	Batch	Spectra
Cloae	Citric oil	18328006	2
Fagron	Citric oil	13K14-B03-294704	1
Fagron	Citric oil	14H06-B02-299949	1
Fagron	Citric oil	14H06-B02-308273	1
Fagron	Citric oil	15F29-804	1
Fagron	Citric oil	15F29-B04	2
Fagron	Citric oil	15F29-B04-322985	1
Fagron	Citric oil	15f29-b04-325354	1
Fagron	Citric oil	15F29-B04-325354	1
Fagron	Citric oil	15F29-B04-330854	1
Fagron	Citric oil	15F9-B04-330854	1
Fagron	Citric oil	17B14-B04	1
Fagron	Citric oil	17B14-B04-334835	1
Fagron	Citric oil	17B14-B04-350559	2
Fagron	Citric oil	17B14-B04-352490	1
Fagron	Citric oil	17B14B04341736	1
Fagron	Citric oil	19K11-F08	1
Gehe	Citric oil	2204097006	1
Gehe	Citric oil	23001006	1
Hänseler	Citric oil		3
Kögl	Citric oil	182006163916	1
Noweda	Citric oil	24001610	1
Noweda	Citric oil	2947IT-K05	1
noweda	Citric oil	P206065	1
noweda	Citric oil	P309047	1
Primavera Life GmbH	Citric oil	81M29	1
Primavera	Citric oil	25K29	1
Primavera	Citric oil	285F28	1
Primavera	Citric oil	462G28	1
Primavera	Citric oil	552K28	1
Primavera	Citric oil	669A30	2
Primavera	Citric oil	96D28	1
Primavera/ Phönix	Citric oil	595G26	1
Primavera/Primavera	Citric oil	669A30	1
Primavera/Primavera	Citric oil	722590	1
Sanacorp	Citric oil	15182703	1
sanacorp	Citric oil	23002829005	1
Taoasis	Citric oil	1/21LM-13639	2
Taoasis	Lime oil	111806-9406	1
Taoasis	Citric oil	3681003-124333	1
Taoasis	Lime oil	867-124956	2
Taoasis	Lime oil	867-127657	1
Taoasis	Citric oil	E160576-127218	1
Taoasis	Citric oil	W160567-127218	1
Taoasis/Sanaorp	Lime oil	867_124704I05	1
Taoasis/Taoasis	Lime oil	867-124956	1

- 20 634 spectra from 1552 *Apo-Ident* customers from a total of 6251 batches from a further 165 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Citric oil* / *Lime oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citric oil* / *Lime oil* and it was

evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	420	0	27 514
Type B	0	340	0	30 590
Type C	0	144	0	20 634

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9614 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9564 %)	100.0000 % (> 98.2353 %)
Type C	100.0000 % (> 99.0585 %)	100.0000 % (> 95.8333 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31544	31544	0.00	33.98
31558	31558	0.00	18.52
31838	31838	0.00	17.45
33611	33611	0.00	17.30
33874	33874	0.00	42.20
33942	33942	0.00	41.72
34393	34393	0.00	30.79
37664	37664	0.00	67.91

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Citronella oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31550-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Citronella oil; Oleum cymbopogon winterianus

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Citronella oil	4	3	15

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citronella oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Rose-geranium oil, organic	22.45	—
Lemon grass oil	31.44	—
Palmarosa oil, organic	39.80	—
Marjoram oil	47.07	—
Patchouli oil	48.26	—
Tea tree oil	48.46	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Citronella oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Citronella oil	00671A27	34409	40	not required
Taoasis	Citronella oil	140121-115623	31550	60	not required
Taoasis	Citronella oil	1291021-122850	31840	60	not required
Taoasis	Citronella oil	1794-373	33728	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 4 reference samples from the substance/substance group *Citronella oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.

- 27734 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Citronella oil	108494-126305	32798	40
Taoasis	Citronella oil	108494-126776	33047	40
Taoasis	Citronella oil	19958	38786	40

- 30810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 16 spectra from 15 *Apo-Ident* customers from 15 batches from the substance/substance group *Citronella oil*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Apotheker Bauer und ...	Citronella oil	7444171705	1
ASAV/Noweda	Citronella oil	1242	1
Bombastus	Citronella oil	18004737	1
Bombastus	Citronella oil	19001887	1
Bombastus	Citronella oil	19003198	1
Bombastus	Citronella oil	19004993	2
Bombastus	Citronella oil	21001777	1
Caelo	Citronella oil	19059006	1
Caelo	Citronella oil	200002042002	1
Caelo	Citronella oil	20003597002	1

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Supplier	Substance	Batch	Spectra
Kögl	Citronella oil	228107163016	1
noweda	Citronella oil	20209031853	1
Phoenix	Citronella oil	16491IDR01	1
Taoasis	Citronella oil	2291-3445	1
Taoasis	Citronella oil	5211028-120284	1

- 20 762 spectra from 1559 *Apo-Ident* customers from a total of 6337 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	120	0	30 810
Type C	0	16	0	20 762

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0613 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31550	31550	0.00	35.50
31840	31840	0.00	39.35
33728	33728	0.00	36.43
34409	34409	0.00	37.27

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group	Citrus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil
Substance class	BR APIs & excipients, liquid/semi-solid (other)
Report date	28/04/2026
Report number	30961-2026-04-28
Executing company	HiperScan GmbH Gerokstraße 13 01307 Dresden Germany

Relevant substance names

Citrus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil; Citrus oil; Clary sage oil; Hyssop oil; Lavender oil; Myrtle oil; Oleum citrus aurantium; Oleum hyssopus officinalis; Oleum lavendula officinalis; Oleum salviae sclarea; Petitgrain oil

Special notes

When selecting the *Citrus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	<i>European Pharmacopoeia 11th Edition, Basic Version 2022</i> [3]
Komm2.2.40	<i>Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident</i> [4]
AA010	<i>Creation of IdentModule Updates</i>

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Citrus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil	28	17	121

Second-stage model

For differentiation of the substance/substance group *Citrus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Neroli oil	19.68	—
Ravintsara oil	19.85	—
Rosemary oil	23.85	—
Immortelle oil	24.90	—
Vetiver bourbon oil	24.93	—
Marjoram oil	24.93	—
Cypress oil	25.88	—
Sage oil	26.32	—
Melissa oil 30%	26.67	—
Thyme oil, white	27.41	—
Angelica root oil	28.19	—
Camphor oil	33.79	—
Cedar wood oil	35.96	—
Rosemary camphor oil	36.13	—
Yarrow oil	41.13	—
Matricaria oil, morrocan	41.16	—
Ginger oil	42.12	—
Bergamot oil	43.05	—
Cumin oil	43.42	—
Niaouli oil	44.18	—
Cajeput (essentiell oil)	46.02	—
Matricaria oil, roman	46.43	—
Ylang-ylang oil	46.55	—
Frankincense oil	47.98	—
Coriander oil	50.56	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained

from the substance/substance group *Citrus oil* / *Lavender oil* / *Clary sage oil* / *Myrtle oil* / *Petitgrain oil* / *Hyssop oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Citrus oil	00438D25	33760	40	not required
Primavera	Citrus oil	00621G26	34294	40	not required
Primavera	Citrus oil	00673L26	34395	40	not required
Taoasis	Citrus oil	788	33816	40	not required
Primavera	Clary sage oil	00529M26	34367	40	not required
Primavera	Clary sage oil	00477M31	37977	40	not required
Taoasis	Clary sage oil	2098-115222	31669	60	not required
Taoasis	Clary sage oil	1834-127059	33033	40	not required
Taoasis	Clary sage oil	019167-14982	37666	40	not required
Apotheker ...	Hyssop oil	13.201345120.16.02	31850	60	not required
Taoasis	Hyssop oil	31823-118643	31649	60	not required
Taoasis	Hyssop oil	33065-122200	31782	60	not required
Taoasis	Hyssop oil	1616260-125049	32980	40	not required
Taoasis	Hyssop oil	7691-17369	37686	40	not required
Primavera	Lavender oil	00684K25	33804	40	not required
Primavera	Lavender oil	00270J31	37783	40	not required
Taoasis	Lavender oil	L16812DN-108661BAG90451	30961	40	not required
Taoasis	Lavender oil	110186BAG90451	30962	40	not required
Taoasis	Lavender oil	22015-121843	31756	60	not required
Taoasis	Lavender oil	17283-BG-R06	37654	40	not required
Taoasis	Lavender oil	19998	38778	40	not required
Primavera	Myrtle oil	00401D25	33797	40	not required
Primavera	Myrtle oil	00877L25	33957	40	not required
Taoasis	Myrtle oil	013	33830	40	not required
Taoasis	Myrtle oil	20771	38783	40	not required
Apotheker ...	Petitgrain oil	6.56267.16.02	31852	60	not required
Taoasis	Petitgrain oil	26056-120864	31778	60	not required
Taoasis	Petitgrain oil	4031015-126048	33024	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1260 spectra of 28 reference samples from the substance/substance group *Citrus oil* / *Lavender oil* / *Clary sage oil* / *Myrtle oil* / *Petitgrain oil* / *Hyssop oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 28 different batches.
- 26 674 spectra from a total of 572 batches from further 138 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra

in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 800 spectra of 20 reference samples from the substance/substance group *Citrus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil*.
- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Citrus oil	00348C26	34178	40
Taoasis	Citrus oil	1510-135	33817	40
Taoasis	Citrus oil	10611-17088	37659	40
Taoasis	Clary sage oil	487962-107805BAG90451	30749	40
Taoasis	Clary sage oil	10140-145	33871	40
Taoasis	Clary sage oil	1834-129098	34284	40
Apotheker Bauer & Cie	Hyssop oil	13.201604082.17.01	32923	40
Taoasis	Hyssop oil	1616260-1982	34110	40
Primavera	Lavender oil	00793A26	33953	40
Primavera	Lavender oil	00184G26	34165	40
Taoasis	Lavender oil	2/2015-125808I09	33015	40
Taoasis	Lavender oil	22015-125925I10	33016	40
Primavera	Myrtle oil	00971J25	33807	40
Primavera	Myrtle oil	00392M26	34384	40
Taoasis	Petitgrain oil	29551-105402BAG90451	30752	40
Taoasis	Petitgrain oil	4031015-147	34108	40
Taoasis	Petitgrain oil	10471-17101	37679	40
Taoasis	Clary sage oil	2098-115222	32797	40
Taoasis	Clary sage oil	10140-145	33943	40
Taoasis	Petitgrain oil	4031015-126048	33025	40

- 30130 spectra from a total of 690 batches from further 205 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 167 spectra from 93 *Apo-Ident* customers from 122 batches from the substance/substance group *Citrus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil*.
- Among them are spectra of independent samples from 121 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Lavender oil	22000129020	1
	Lavender oil	23000801	1
	Lavender oil	23003503002	1
	Lavender oil	CA47A	1
	Lavender oil	P307002	1
00342304	Lavender oil	750E30	1
Alliance	Lavender oil	444C32	1

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Supplier	Substance	Batch	Spectra
bergl	Lavender oil	K704066	1
Bergland-Pharma/Phönix	Lavender oil	P107037	1
Bergland	Lavender oil	K502790	1
Bergland	Lavender oil	K704088	1
Bombastus	Lavender oil	18000582	1
Bombastus	Lavender oil	19001102	2
Bombastus	Lavender oil	19004002	1
Bombastus	Lavender oil	19004173	1
Bombastus	Lavender oil	20003765	1
Bombastus	Lavender oil	20004664	1
Bombastus	Lavender oil	21000345	1
Bombastus	Lavender oil	21001285	1
Bombastus	Lavender oil	21002770	1
Bombastus	Lavender oil	21003530	1
Bombastus	Lavender oil	22004192	1
Bombastus	Lavender oil	277818	1
Bombastus	Lavender oil	300666	1
Bombastus	Lavender oil	303303	1
Bombastus	Lavender oil	305279	1
Bombastus	Lavender oil	306049	1
Bombastus	Lavender oil	310024	1
Bombastus	Lavender oil	80311204	1
Bombastus /Jenne	Lavender oil	310024	1
Caelo	Lavender oil	1010548	2
Caelo	Lavender oil	15278105	1
Caelo	Lavender oil	16023001	1
Caelo	Lavender oil	16023017	1
Caelo	Lavender oil	16292205	1
Caelo	Lavender oil	16292211	2
Caelo	Lavender oil	16292214	1
Caelo	Lavender oil	16292216	2
Caelo	Lavender oil	17132711	5
Caelo	Lavender oil	18128202	2
Caelo	Lavender oil	18128203	1
Caelo	Lavender oil	18128204	2
Caelo	Lavender oil	18219005	1
Caelo	Lavender oil	18219011	2
Caelo	Lavender oil	18219012	1
Caelo	Lavender oil	18326213	1
Caelo	Lavender oil	18b26b02352705	1
Caelo	Lavender oil	191847007	1
Caelo	Lavender oil	191847010	1
Caelo	Lavender oil	20001640007	1
Caelo	Lavender oil	21001627009	1
Caelo	Lavender oil	21001627014	1
Caelo	Lavender oil	21001627016	1
Caelo	Lavender oil	22000129006	1
Caelo	Lavender oil	8259FR-L10	1
Caesar & Loretz GmbH	Lavender oil	20003808010	1
Cordes/Noweda	Lavender oil	16023002	1
Euro OTC	Lavender oil	1706003-01	1
Euro OTC	Lavender oil	1710038-02	1
Fagron	Lavender oil	1061076	1
Fagron	Lavender oil	16H01-B04	1
Fagron	Lavender oil	17G20-B07-342691	2
Fagron	Lavender oil	18K19-B01	1
Fagron	Lavender oil	19B20-B01-191698	1
Gehe	Lavender oil	22004095014	1
Noweda	Lavender oil	23001734	1
PHOENIX	Lavender oil	23000801	1

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Supplier	Substance	Batch	Spectra
Phönix	Lavender oil	1177388	1
Phönix	Lavender oil	24002287	1
Phönix	Lavender oil	P209017	1
Primavera, Gehe	Lavender oil	21A27	1
Primavera, Gehe	Lavender oil	220L27	1
Primavera, Gehe	Lavender oil	285H25	1
Primavera	Lavender oil	1078C23	1
Primavera	Lavender oil	209L29	1
Primavera	Lavender oil	408B29	1
Primavera	Lavender oil	471A27	1
Primavera	Lavender oil	648C28	1
Primavera	Citus oil	673L26	1
Primavera/Noweda	Lavender oil	378E25	1
Primavera/Phoenix	Lavender oil	326C26	1
Primavera/Primavera	Lavender oil	50A30	1
Ssanacorp	Lavender oil	23003503001	1
Taoasis	Clary sage oil	10140-146	1
Taoasis	Lavender oil	10227IT-M07	1
Taoasis	Lavender oil	106082301/2016-2909	1
Taoasis	Lavender oil	109744-6805	1
Taoasis	Lavender oil	110647-7297	1
Taoasis	Myrtle oil	116344-13884	2
Taoasis	Clary sage oil	13304-5798	2
Taoasis	Clary sage oil	13304-6656	1
Taoasis	Citus oil	1510-1171	1
Taoasis	Lavender oil	160802301/2016-1909	1
Taoasis	Lavender oil	16082301/2016-2908	1
Taoasis	Lavender oil	16082301/2016-2909	4
Taoasis	Lavender oil	16082301/2016/2908	1
Taoasis	Clary sage oil	1700-125289	2
Taoasis	Lavender oil	170001022016-5298	1
Taoasis	Lavender oil	170124022016-5298	1
Taoasis	Lavender oil	2/2015-125808I09	12
Taoasis	Lavender oil	2015-2394	3
Taoasis	Clary sage oil	2098-115222	1
Taoasis	Clary sage oil	2098-119159	1
Taoasis	Lavender oil	22015-125927	2
Taoasis	Lavender oil	22015-126998	3
Taoasis	Lavender oil	22015-128587	1
Taoasis	Lavender oil	22015-508	5
Taoasis	Citus oil	2345-2578	2
Taoasis	Hyssop oil	31095-105392	1
Taoasis	Lavender oil	34/151/16	1
Taoasis	Lavender oil	4651010	1
Taoasis	Clary sage oil	487962-106655	1
Taoasis	Lavender oil	6981BG-L05	1
Taoasis	Lavender oil	96336-5473	2
Taoasis	Lavender oil	RM20_13642	1
Taoasis	Lavender oil	S05-18-6464	3
Taoasis	Lavender oil	S0519-10410	1
Taoasis	Lavender oil	S0519-11000	1
Taoasis/AHD	Lavender oil	13422BG-N09	1
Taoasis/Noweda	Lavender oil	16716-126380/11	1
Taoasis/Phoenix/10.0...	Lavender oil	5083	1
Taoasis/Taoasis	Lavender oil	L665-5037	1
Wadi	Lavender oil	180620-005696	2
Wadi	Lavender oil	51119-005330	1

- 20611 spectra from 1554 *Apo-Ident* customers from a total of 6230 batches from a further 162

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

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	1260	0	26 674
Type B	0	790	10	30 130
Type C	0	167	0	20 611

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9613 %)	100.0000 % (> 99.5238 %)
Type B	100.0000 % (> 99.9564 %)	98.7500 % (> 98.3750 %)
Type C	100.0000 % (> 99.0585 %)	100.0000 % (> 96.4072 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30961	30961	0.00	50.56
30962	30962	0.00	62.24
31649	31649	0.00	41.13
31669	31669	0.00	46.55
31756	31756	0.00	68.59
31778	31778	0.00	64.49
31782	31782	0.00	42.26
31850	31850	0.00	43.05
31852	31852	0.00	28.14

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
32980	32980	0.00	19.85
33024	33024	0.00	57.57
33033	33033	0.00	48.45
33760	33760	0.00	36.33
33797	33797	0.00	33.34
33804	33804	0.00	67.20
33816	33816	0.00	35.66
33830	33830	0.00	44.46
33957	33957	0.00	34.08
34294	34294	0.00	33.33
34367	34367	0.00	68.77
34395	34395	0.00	32.00
37654	37654	0.00	60.77
37666	37666	0.00	48.22
37686	37686	0.00	26.00
37783	37783	0.00	50.51
37977	37977	0.00	49.60
38778	38778	0.00	48.72
38783	38783	0.00	45.31

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Clove oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31270-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Clove oil; Oleum caryophylli

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Clove oil	4	2	21

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Clove oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Siam benzoin (solution)	381.96	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Clove oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Bombastus	Clove oil	279132	31035	40	not required
Caelo	Clove oil	12380605	31270	40	not required
Taoasis	Clove oil	2891012-116936	31557	60	not required
Taoasis	Clove oil	1426-120481	31683	60	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 4 reference samples from the substance/substance group *Clove oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 734 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by

this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 3 reference samples from the substance/substance group *Clove oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Clove oil	1598-124689	32938	40
Taoasis	Clove oil	19948	38592	40
Taoasis	Clove oil	1598-124689	32940	40

- 30810 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 24 spectra from 20 *Apo-Ident* customers from 21 batches from the substance/substance group *Clove oil*.
- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Clove oil	22002227006	1
	Clove oil	22002227009	3
	Clove oil	497D32	1
Caelo	Clove oil	15119304	1
Caelo	Clove oil	15316102	1
Caelo	Clove oil	15316103	1
Caelo	Clove oil	15402108	1
Caelo	Clove oil	15402109	1
Caelo	Clove oil	17354205	2
Caelo	Clove oil	18178005	1
Caelo	Clove oil	19066804	1
Caelo	Clove oil	19066809	1
Caelo	Clove oil	21002670011	1
Caesar & Loretz GmbH...	Clove oil	20003989004	1

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Supplier	Substance	Batch	Spectra
Primavera	Clove oil	329C30	1
Primavera	Clove oil	377F30	1
Primavera	Clove oil	47G24	1
Primavera/Primavera	Clove oil	31L29	1
Primavera/Primavera	Clove oil	397B29	1
Primavera/Sanacorp	Clove oil	133A25	1
Taoasis	Clove oil	2638-7673	1

- 20 754 spectra from 1558 *Apo-Ident* customers from a total of 6331 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	120	0	30 810
Type C	0	22	2	20 754

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0603 %)	91.6667 % (> 79.1667 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31035	31035	0.00	435.89
31270	31270	0.00	436.92
31557	31557	0.00	422.47
31683	31683	0.00	428.73

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Contramarum aroma**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31007-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Contramarum aroma; Contramarum flavour

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Contramarum aroma	6	5	106

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Contramarum aroma* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Raspberry aroma	40.24	—
Strawberry aroma	79.94	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Contramarum aroma*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Contramarum aroma	13141605	31007	40	1403096
Caelo	Contramarum aroma	13411002	31289	40	not required
Caelo	Contramarum aroma	13411007	31398	40	not required
Caelo	Contramarum aroma	21002097002	35897	50	not required
Caelo	Contramarum aroma	22000814003	36582	40	not required
Caelo	Contramarum aroma	23000302002	37456	30	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 6 reference samples from the substance/substance group *Contramarum aroma*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 6 different batches.

- 27 694 spectra from a total of 594 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Contramarum aroma	162671	32695	40
Caelo	Contramarum aroma	172230	33701	40
Caelo	Contramarum aroma	181067	34066	40
Caelo	Contramarum aroma	23003242	38417	40
Caelo	Contramarum aroma	24002454	38730	40

- 30 730 spectra from a total of 704 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 328 spectra from 132 *Apo-Ident* customers from 109 batches from the substance/substance group *Contramarum aroma*.
- Among them are spectra of independent samples from 106 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Contramarum aroma	22002935001	2
	Contramarum aroma	22002935002	2
	Contramarum aroma	22002935003	1
	Contramarum aroma	23000302004	1
	Contramarum aroma	23001561001	7
	Contramarum aroma	23001561002	2
	Contramarum aroma	23003242001	1
	Contramarum aroma	23003242002	2

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Supplier	Substance	Batch	Spectra
AHC	Contramarum aroma	24000815001	2
	Contramarum aroma	24000815002	3
Alliance Healthcare	Contramarum aroma	24002454001	1
	Contramarum aroma	24002454002	3
Cael	Contramarum aroma	23001561001	1
	Contramarum aroma	17223007	1
Caelo	Contramarum aroma	13141603	1
	Contramarum aroma	11378804	1
Caelo	Contramarum aroma	12051808	1
	Contramarum aroma	12201407	2
Caelo	Contramarum aroma	13141606	3
	Contramarum aroma	13141608	2
Caelo	Contramarum aroma	1315Q-03148	1
	Contramarum aroma	13411007	4
Caelo	Contramarum aroma	13411008	1
	Contramarum aroma	13411011	1
Caelo	Contramarum aroma	134111002	1
	Contramarum aroma	13815152	1
Caelo	Contramarum aroma	143200009	1
	Contramarum aroma	14320001	1
Caelo	Contramarum aroma	14320005	1
	Contramarum aroma	14320006	3
Caelo	Contramarum aroma	14320008	1
	Contramarum aroma	14320009	2
Caelo	Contramarum aroma	14320015	3
	Contramarum aroma	15113002	3
Caelo	Contramarum aroma	15113003	2
	Contramarum aroma	15113011	1
Caelo	Contramarum aroma	16083801	9
	Contramarum aroma	16083802	2
Caelo	Contramarum aroma	16083804	2
	Contramarum aroma	16083805	1
Caelo	Contramarum aroma	16083806	1
	Contramarum aroma	16267101	7
Caelo	Contramarum aroma	16267102	4
	Contramarum aroma	16267103	6
Caelo	Contramarum aroma	169267103	1
	Contramarum aroma	17223001	9
Caelo	Contramarum aroma	17223002	6
	Contramarum aroma	17223004	4
Caelo	Contramarum aroma	17223005	5
	Contramarum aroma	17223007	7
Caelo	Contramarum aroma	17223008	2
	Contramarum aroma	18106701	1
Caelo	Contramarum aroma	18106702	8
	Contramarum aroma	18106703	12
Caelo	Contramarum aroma	18106705	1
	Contramarum aroma	18106706	2
Caelo	Contramarum aroma	19065401	12
	Contramarum aroma	19065403	5
Caelo	Contramarum aroma	19121701	1
	Contramarum aroma	19129001	4
Caelo	Contramarum aroma	19129002	3
	Contramarum aroma	192009401	1
Caelo	Contramarum aroma	19209401	6
	Contramarum aroma	19209402	2
Caelo	Contramarum aroma	19209403	3
	Contramarum aroma	192867003	5
Caelo	Contramarum aroma	192867004	1
	Contramarum aroma	192867005	2

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Supplier	Substance	Batch	Spectra
Caelo	Contramarum aroma	192867006	1
Caelo	Contramarum aroma	20(16267103)	1
Caelo	Contramarum aroma	2000061002	1
Caelo	Contramarum aroma	20000961002	5
Caelo	Contramarum aroma	20000961003	3
Caelo	Contramarum aroma	20000961005	1
Caelo	Contramarum aroma	20002656001	3
Caelo	Contramarum aroma	20002656002	2
Caelo	Contramarum aroma	20002656005	1
Caelo	Contramarum aroma	20002656006	3
Caelo	Contramarum aroma	20004334002	3
Caelo	Contramarum aroma	2041515	1
Caelo	Contramarum aroma	21(17223001)	1
Caelo	Contramarum aroma	21002097001	2
Caelo	Contramarum aroma	21002097002	3
Caelo	Contramarum aroma	21002097003	2
Caelo	Contramarum aroma	21002097004	1
Caelo	Contramarum aroma	21003710001	1
Caelo	Contramarum aroma	21003710003	4
Caelo	Contramarum aroma	2100371003	1
Caelo	Contramarum aroma	21051508	1
Caelo	Contramarum aroma	22(18106701)	1
Caelo	Contramarum aroma	22000814001	2
Caelo	Contramarum aroma	22000814002	3
Caelo	Contramarum aroma	22002935001	1
Caelo	Contramarum aroma	22002935002	1
Caelo	Contramarum aroma	22002935003	1
Caelo	Contramarum aroma	23(19065401)	1
Caelo	Contramarum aroma	24(20000961002)	1
Caelo	Contramarum aroma	26267101	1
Caelo	Contramarum aroma	30081804	1
Caelo	Contramarum aroma	4916E-03148	1
Caelo	Contramarum aroma	5315A-03148	1
Caelo	Contramarum aroma	7071207	1
Caelo	Contramarum aroma	7082006	1
Caelo	Contramarum aroma	7091302	1
Caelo	Contramarum aroma	P-31071921/19129001	1
Caesar & Loretz /AHD	Contramarum aroma	21002097002	1
Caesar & Loretz GmbH ...	Contramarum aroma	22002935001	1
Caesar & Loretz GmbH	Contramarum aroma	18106702	1
Caesar & Loretz GmbH	Contramarum aroma	19065401	3
Caesar & Loretz GmbH	Contramarum aroma	19065403	5
Caesar & Loretz GmbH	Contramarum aroma	19129001	2
Caesar & Loretz GmbH	Contramarum aroma	19129002	1
Caesar & Loretz GmbH	Contramarum aroma	19209401	1
Caesar & Loretz GmbH	Contramarum aroma	19209402	1
Caesar & Loretz GmbH	Contramarum aroma	19209403	2
Caesar & Loretz GmbH	Contramarum aroma	192867003	1
Caesar & Loretz GmbH	Contramarum aroma	192867004	1
Caesar & Loretz GmbH	Contramarum aroma	192867006	2
Caesar & Loretz GmbH	Contramarum aroma	20000961002	1
Caesar & Loretz GmbH	Contramarum aroma	20000961004	1
Caesar & Loretz GmbH	Contramarum aroma	20000961005	2
Caesar & Loretz GmbH	Contramarum aroma	20002656001	2
Caesar & Loretz GmbH	Contramarum aroma	20002656002	2
Caesar & Loretz GmbH	Contramarum aroma	20004334003	1
Caesar & Loretz GmbH	Contramarum aroma	21002097001	1
Caesar & Loretz GmbH	Contramarum aroma	21002097002	3
Caesar & Loretz GmbH	Contramarum aroma	21003710001	1
Caesar & Loretz GmbH	Contramarum aroma	22000814004	2

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Contramarum aroma	22002935001	1
Caesar & Loretz GmbH	Contramarum aroma	22002935002	3
Caesar & Loretz GmbH...	Contramarum aroma	192867004	1
Caesar & Loretz GmbH...	Contramarum aroma	20004334002	1
Caesar & Loretz GmbH...	Contramarum aroma	20000961002	1
Caesar & Loretz GmbH/Gehe	Contramarum aroma	21003710001	1
Caesar & Loretz GmbH/Gehe	Contramarum aroma	23000302002	1
Caesar & Loretz GmbH...	Contramarum aroma	21002097003	1
Caesar & Loretz GmbH...	Contramarum aroma	19065401	1
Caesar & Loretz GmbH...	Contramarum aroma	20000961004	1
Caesar & Loretz GmbH...	Contramarum aroma	20004334004	1
Caesar & Loretz GmbH...	Contramarum aroma	21003710001	1
Caesar & Loretz GmbH...	Contramarum aroma	192867004	1
Fagron	Contramarum aroma	16083801	1
Fiebig	Contramarum aroma	11378810	1
Gehe	Contramarum aroma	12201404	1
Gehe	Contramarum aroma	20000961002	1
Gehe	Contramarum aroma	24000815001	1
Noweda	Contramarum aroma	23000302002	1
Noweda	Contramarum aroma	23003242001	1
Phoenix Goettin	Contramarum aroma	70401432001	1
Phönix	Contramarum aroma	17223007	1
Phönix	Contramarum aroma	20000961004	1
Phönix	Contramarum aroma	20004334003	1
Phönix	Contramarum aroma	20004334005	1
VDL; 18.07.15; 6,56EUR	Contramarum aroma	14320005	1
VDL;02.01.15;6,42EUR	Contramarum aroma	14320001	1

- 20 450 spectra from 1545 *Apo-Ident* customers from a total of 6243 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	240	0	27 694
Type B	0	200	0	30 730
Type C	0	327	1	20 450

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.0583 %)	99.6951 % (> 98.7805 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31007	31007	0.00	59.64
31289	31289	0.00	55.75
31398	31398	0.00	58.51
35897	35897	0.00	59.09
36582	36582	0.00	58.14
37456	37456	0.00	60.89

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Cumin oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30449-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Cumin oil; Oleum cuminum cyminum

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Cumin oil	3	2	4

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cumin oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	79.94	–

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Cumin oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Cumin oil	130910-113031BAG90451	31141	40	not required
Taoasis	Cumin oil	51764-124375	32267	40	not required
Taoasis	Cumin oil	51764-124375	32904	40	not required
Taoasis	Cumin oil	18831	38593	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Cumin oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.
- 27 774 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by

this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 3 reference samples from the substance/substance group *Cumin oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Cumin oil	2016109952-127656	33841	40
Taoasis	Cumin oil	2016109952-128855	33873	40
Taoasis	Cumin oil	51764-124375	32266	40

- 30810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

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

Supplier	Substance	Batch	Spectra
Taoasis	Cumin oil	104723-298	1
Taoasis	Cumin oil	121217-111221	1
Taoasis	Cumin oil	24081-106027	1
Taoasis/Noweda	Cumin oil	51764-124373BAG9045	1

- 20774 spectra from 1559 *Apo-Ident* customers from a total of 6348 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	160	0	27 774
Type B	0	120	0	30 810
Type C	0	4	0	20 774

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9618 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0708 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31141	31141	0.00	134.90
32267	32267	0.00	132.29
32904	32904	0.00	137.36
38593	38593	0.00	127.06

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Cypress oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30457-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Cypress oil; Oleum cupressus sempervirens

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Cypress oil	5	3	17

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cypress oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	23.19	—
Citus oil	28.47	—
Myrtle oil	33.57	—
Immortelle oil	37.40	—
Dwarf pine oil	39.94	—
Vetiver bourbon oil	44.70	—
Hyssop oil	45.09	—
Cumin oil	45.85	—
Ginger oil	49.40	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Cypress oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Cypress oil	00177G25	33802	40	not required
Primavera	Cypress oil	00403L25	33954	40	not required
Taoasis	Cypress oil	732-119820	31656	60	not required
Taoasis	Cypress oil	43953-129229	33623	40	not required
Taoasis	Cypress oil	10032-16978	37678	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 5 reference samples from the substance/substance group *Cypress oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27714 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 160 spectra of 4 reference samples from the substance/substance group *Cypress oil*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Cypress oil	00586C26	34169	40
Primavera	Cypress oil	00660L26	34394	40
Taoasis	Cypress oil	107527-125443	32806	40
Taoasis	Cypress oil	107527-125443	33045	40

- 30770 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 27 spectra from 5 *Apo-Ident* customers from 18 batches from the substance/substance group *Cypress oil*.
- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cypress oil	17031	1
Primavera	Cypress oil	431C27	1
Taoasis	Cypress oil	1039-121894	3
Taoasis	Cypress oil	1039-122434	1
Taoasis	Cypress oil	107527-125443	2

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Supplier	Substance	Batch	Spectra
Taoasis	Cypress oil	107527-125965	1
Taoasis	Cypress oil	107527-127323	6
Taoasis	Cypress oil	107527-27014	1
Taoasis	Cypress oil	33720-115882	1
Taoasis	Cypress oil	33720-118623	1
Taoasis	Cypress oil	33720-118895	2
Taoasis	Cypress oil	341012-123298	1
Taoasis	Cypress oil	43953-129229	1
Taoasis	Cypress oil	45953-129229	1
Taoasis	Cypress oil	487749-107790	1
Taoasis	Cypress oil	487749-108547	1
Taoasis	Cypress oil	514085-111139	1
Taoasis	Cypress oil	6483-12594	1

- 20 751 spectra from 1559 *Apo-Ident* customers from a total of 6334 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	220	0	27 714
Type B	0	153	7	30 770
Type C	0	27	0	20 751

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9565 %)	95.6250 % (> 93.7500 %)
Type C	100.0000 % (> 99.0601 %)	100.0000 % (> 77.7778 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31656	31656	0.00	63.01
33623	33623	0.00	64.94
33802	33802	0.00	47.03
33954	33954	0.00	45.09
37678	37678	0.00	65.46

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Dichloroacetic acid**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 10005427-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Dichloroacetic acid; Acidum dichloroaceticum

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Dichloroacetic acid	3	1	0

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dichloroacetic acid* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Nicotine	192.01	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Dichloroacetic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Merck	Dichloroacetic acid	S6674841451	31642	60	not required
Merck	Dichloroacetic acid	S7209041737	33794	40	not required
Merck	Dichloroacetic acid	S7209241824	34185	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 3 reference samples from the substance/substance group *Dichloroacetic acid*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.
- 27 794 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for

model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Merck	Dichloroacetic acid	S6674841614	32750	40

- 30 890 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Dichloroacetic acid*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 20 778 spectra from 1559 *Apo-Ident* customers from a total of 6352 batches from a further 167 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	140	0	27 794
Type B	0	40	0	30 890
Type C	0	0	0	20 778

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9618 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9570 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.0752 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31642	31642	0.00	245.14
33794	33794	0.00	277.33
34185	34185	0.00	261.39

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Dimeticone ointment 10% SR**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31243-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Dimeticone ointment 10% SR; Unguentum dimeticoni 10% SR

Special notes

When selecting the *Dimeticone ointment 10% SR* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Dimeticone ointment 10% SR	3	5	49

Second-stage model

For differentiation of the substance/substance group *Dimeticone ointment 10% SR* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dimeticone ointment 10% SR* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Hans Karrer Lipolotion MicroSilver	13.70	—
Asche Basis [®] lotion	21.43	—
Base cream Taoasis	22.52	—
Excipial [®] U Lipolotio	26.80	—
DMS [®] base cream classic	26.90	—
DMS [®] base cream high classic	27.47	—
Hans Karrer Lipocream MicroSilver	27.84	—
Excipial [®] U10 Lipolotio	29.25	—
Dexeryl [®]	29.63	—
Abitima [®] clinic body cream	33.43	—
ALLERGIKA [®] – Face cream MED	34.18	—
Neribas [®] cream	35.84	—
Abitima [®] clinic face cream	38.63	—
Neuroderm [®] care lotion	39.17	—
Linola [®] body milk	39.46	—
Fabitop [®] base cream	39.59	—
Neuroderm [®] moisturising cream	41.00	—
Asche Basis [®] cream	44.15	—
DMS [®] base cream high classic plus	48.93	—
Ultrasicc [®]	49.04	—
Excipial [®] hydro cream	51.38	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dimeticone ointment 10% SR* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Dimeticone ointment 10% SR*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
apomix	Dimeticone ointment 10% SR	08B041213	31243	30	not required
apomix	Dimeticone ointment 10% SR	10A181214	31638	60	not required
apomix	Dimeticone ointment 10% SR	11A271216	33041	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 130 spectra of 3 reference samples from the substance/substance group *Dimeticone ointment 10% SR*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.
- 27 804 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 200 spectra of 5 reference samples from the substance/substance group *Dimeticone ointment 10% SR*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
apomix	Dimeticone ointment 10% SR	10A021117	33870	40
apomix	Dimeticone ointment 10% SR	02A150322	36234	40
apomix	Dimeticone ointment 10% SR	01A010223	36905	40
apomix	Dimeticone ointment 10% SR	06A221123	37947	40
apomix	Dimeticone ointment 10% SR	01A200125	38769	40

- 30 730 spectra from a total of 704 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 85 spectra from 20 *Apo-Ident* customers from 51 batches from the substance/substance group *Dimeticone ointment 10% SR*.
- Among them are spectra of independent samples from 49 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
apomix	Dimeticone ointment 10% SR	1A060324	3
	Dimeticone ointment 10% SR	2A020425	1
	Dimeticone ointment 10% SR	2A200423	4
	Dimeticone ointment 10% SR	3A130723	2
	Dimeticone ointment 10% SR	4A140524	1
	Dimeticone ointment 10% SR	4A170822	1
	Dimeticone ointment 10% SR	4A231023	2
	Dimeticone ointment 10% SR	4A290425	1
	Dimeticone ointment 10% SR	5A180624	1
	Dimeticone ointment 10% SR	7A010824	1
	Dimeticone ointment 10% SR	10A181214	1
	Dimeticone ointment 10% SR	11a271216	1
	Dimeticone ointment 10% SR	11B031117	1
	Dimeticone ointment 10% SR	1A070121	2
	Dimeticone ointment 10% SR	1A070217	1
	Dimeticone ointment 10% SR	1A120116	1
	Dimeticone ointment 10% SR	1A150115	1
	Dimeticone ointment 10% SR	1A150119	2
	Dimeticone ointment 10% SR	1A210222	2
	Dimeticone ointment 10% SR	1B140120	1
	Dimeticone ointment 10% SR	2A150322	3
	Dimeticone ointment 10% SR	2A180220	2
	Dimeticone ointment 10% SR	2A260219	1
	Dimeticone ointment 10% SR	2B150317	1
	Dimeticone ointment 10% SR	3A220316	1
	Dimeticone ointment 10% SR	3A250522	2
	Dimeticone ointment 10% SR	3B040320	1
	Dimeticone ointment 10% SR	3B180214	1
	Dimeticone ointment 10% SR	4A010415	1
	Dimeticone ointment 10% SR	4A080414	1
	Dimeticone ointment 10% SR	4A170822	2
	Dimeticone ointment 10% SR	4A230519	2
	Dimeticone ointment 10% SR	4C110521	1
	Dimeticone ointment 10% SR	5A020616	1
	Dimeticone ointment 10% SR	5A130520	1
	Dimeticone ointment 10% SR	5A200619	2
	Dimeticone ointment 10% SR	5A210618	3
	Dimeticone ointment 10% SR	6A151222	2
	Dimeticone ointment 10% SR	6A190614	1
	Dimeticone ointment 10% SR	6A300616	1
	Dimeticone ointment 10% SR	7A151019	1
	Dimeticone ointment 10% SR	7A170816	1
	Dimeticone ointment 10% SR	7A310718	1
	Dimeticone ointment 10% SR	7C190820	1
	Dimeticone ointment 10% SR	8A041213	1
	Dimeticone ointment 10% SR	8A090915	1
	Dimeticone ointment 10% SR	9A051218	1
	Dimeticone ointment 10% SR	9A281221	1
	Dimeticone ointment 10% SR	9B041017	1
	Dimeticone ointment 10% SR	3B180214	2

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Supplier	Substance	Batch	Spectra
Holdermann	Dimeticone ointment 10% SR	1A010223	1
Holdermann	Dimeticone ointment 10% SR	4A140524	2
Kehr Holdermann	Dimeticone ointment 10% SR	1A010223	1
Kehr Holdermann	Dimeticone ointment 10% SR	1A060324	1
Kehr	Dimeticone ointment 10% SR	1A200125	1
Noweda	Dimeticone ointment 10% SR	2A200423	1
Phoenix	Dimeticone ointment 10% SR	4A231023	1
Phönix	Dimeticone ointment 10% SR	3A130723	1
Phönix	Dimeticone ointment 10% SR	5A180624	1
Phönix	Dimeticone ointment 10% SR	7A010824	1
PKH GmbH Halle	Dimeticone ointment 10% SR	4A170822	1
PKH GmbH	Dimeticone ointment 10% SR	4A170822	1
PKH Halle	Dimeticone ointment 10% SR	1A310118	1

- 20 693 spectra from 1556 *Apo-Ident* customers from a total of 6301 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Dimeticone ointment 10% SR* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dimeticone ointment 10% SR* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	130	0	27 804
Type B	0	200	0	30 531
Type C	0	85	0	20 693

The substance/substance group *Dimeticone ointment 10% SR* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9619 %)	100.0000 % (> 95.3846 %)
Type B	100.0000 % (> 99.9563 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.0588 %)	100.0000 % (> 92.9412 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31243	31243	0.00	17.43
31638	31638	0.00	18.52
33041	33041	0.00	17.22

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Dwarf pine oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31542-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Dwarf pine oil; Oleum pini pumilionis

Special notes

When selecting the *Dwarf pine oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Dwarf pine oil	5	3	7

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dwarf pine oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Angelica root oil	12.33	—
Spruce needle oil	15.25	—
Cypress oil	15.69	—
Juniper berry oil	19.96	—
Spearmint oil	23.00	—
Frankincense oil	23.53	—
Pine silvestris oil	27.54	—
Swiss pine oil	32.64	—
Silver fir oil	39.13	—
Ginger oil	41.42	—
Marjoram oil	43.95	—
Cumin oil	44.98	—
Citrus oil	48.97	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Dwarf pine oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Dwarf pine oil	586-116867	31542	60	not required
Taoasis	Dwarf pine oil	25599-120877	31689	60	not required
Taoasis	Dwarf pine oil	8783-127273	32937	40	not required
Taoasis	Dwarf pine oil	11148-1980	34109	40	not required
Taoasis	Dwarf pine oil	PM121-17005	37682	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Dwarf pine oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 694 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Dwarf pine oil	00386M26	34377	40
Taoasis	Dwarf pine oil	8783-125163	32811	40
Taoasis	Dwarf pine oil	13260-3453	34290	40

- 30 810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 13 spectra from 5 *Apo-Ident* customers from 8 batches from the substance/substance group *Dwarf pine oil*.
- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Dwarf pine oil	2109024-01	1
Taoasis	Dwarf pine oil	11148-1980	1
Taoasis	Dwarf pine oil	6635-122703	1
Taoasis	Dwarf pine oil	8238-124968	1
Taoasis	Dwarf pine oil	8238-126318	1
Taoasis	Dwarf pine oil	8783-125163	5
Taoasis	Dwarf pine oil	8783-127332	2
Taoasis/Taoasis	Dwarf pine oil	25599120877	1

- 20 765 spectra from 1559 *Apo-Ident* customers from a total of 6344 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	240	0	27 694
Type B	0	120	0	30 810
Type C	0	13	0	20 765

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0621 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31542	31542	0.00	17.09
31689	31689	0.00	15.25
32937	32937	0.00	19.97
34109	34109	0.00	20.24
37682	37682	0.00	32.64

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Ethanol 70%**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30779-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Ethanol 70%; Ethanolum 70%

Special notes

When selecting the *Ethanol 70%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Ethanol 70%	5	4	713

Second-stage model

For differentiation of the substance/substance group *Ethanol 70%* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ethanol 70%* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Orange aroma	52.54	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ethanol 70%* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Ethanol 70%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
apomix	Ethanol 70%	54A170613	31055	40	not required
apomix	Ethanol 70%	08A060618	34274	40	not required
apomix	Ethanol 70%	01A200125	38759	40	not required
Hofmann's	Ethanol 70%	271012	30779	80	1402563
Kremer Gmb...	Ethanol 70%	171211	34101	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Ethanol 70%*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 694 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are

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

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

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

- 160 spectra of 4 reference samples from the substance/substance group *Ethanol 70%*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
apomix	Ethanol 70%	01A020117	33217	40
apomix	Ethanol 70%	09A280322	36245	40
Hofmann's	Ethanol 70%	570916	32591	40
Hofmann's	Ethanol 70%	750718	34317	40

- 30 770 spectra from a total of 705 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1051 spectra from 299 *Apo-Ident* customers from 725 batches from the substance/substance group *Ethanol 70%*.
- Among them are spectra of independent samples from 710 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ethanol 70%		1
	Ethanol 70%	1070123	1
	Ethanol 70%	1080223	1
	Ethanol 70%	1090423	1
	Ethanol 70%	1100723	3
	Ethanol 70%	1110723	1
	Ethanol 70%	1121223	1
	Ethanol 70%	1140324	2
	Ethanol 70%	1150324	1
	Ethanol 70%	1160524	4
	Ethanol 70%	1170524	1
	Ethanol 70%	1191224	1

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Supplier	Substance	Batch	Spectra
	Ethanol 70%	1225I-02320	1
	Ethanol 70%	1225Q-03043	1
	Ethanol 70%	1323A-02320	1
	Ethanol 70%	1325A-02320	1
	Ethanol 70%	145002	1
	Ethanol 70%	145003	1
	Ethanol 70%	1524U-02320	1
	Ethanol 70%	1525E-02320	1
	Ethanol 70%	1624I-02320	1
	Ethanol 70%	1724A-02320	1
	Ethanol 70%	19A16024	1
	Ethanol 70%	2-290725	1
	Ethanol 70%	2023E-02320	1
	Ethanol 70%	21452022	3
	Ethanol 70%	2223Q-02320	1
	Ethanol 70%	2225Q-02320	1
	Ethanol 70%	2225U-03043	1
	Ethanol 70%	225M-02320	1
	Ethanol 70%	2262402	1
	Ethanol 70%	230131	1
	Ethanol 70%	230223	1
	Ethanol 70%	230523	1
	Ethanol 70%	230809H3	1
	Ethanol 70%	230809H4	1
	Ethanol 70%	240322	2
	Ethanol 70%	240729	1
	Ethanol 70%	250324	1
	Ethanol 70%	251125-01	1
	Ethanol 70%	2623E-02320	1
	Ethanol 70%	2625I-02320	1
	Ethanol 70%	2625M-02320	1
	Ethanol 70%	2723M-02320	1
	Ethanol 70%	2823Q-02320	1
	Ethanol 70%	2824M-02320	1
	Ethanol 70%	2923M-02320	1
	Ethanol 70%	324M-02320	1
	Ethanol 70%	325Q-02320	1
	Ethanol 70%	3523A-02320	1
	Ethanol 70%	3523M-02320	1
	Ethanol 70%	3524Q-02320	1
	Ethanol 70%	3625A-02320	1
	Ethanol 70%	3924E-02320	1
	Ethanol 70%	4323A-02320	1
	Ethanol 70%	4325E-02320	1
	Ethanol 70%	4524I-02320	1
	Ethanol 70%	4623E-02320	1
	Ethanol 70%	4624M-02320	1
	Ethanol 70%	4625E-03043	1
	Ethanol 70%	4823A-02320	1
	Ethanol 70%	4923Q-2320	1
	Ethanol 70%	7020101	1
	Ethanol 70%	7021102	1
	Ethanol 70%	7021111	1
	Ethanol 70%	7021112	1
	Ethanol 70%	7022102	2
	Ethanol 70%	7023011	2
	Ethanol 70%	7023021	2
	Ethanol 70%	7023022	4
	Ethanol 70%	7023031	1
	Ethanol 70%	7023033	2

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Supplier	Substance	Batch	Spectra
	Ethanol 70%	7023051	1
	Ethanol 70%	7023063	1
	Ethanol 70%	7023092	4
	Ethanol 70%	7023102	2
	Ethanol 70%	7023111	1
	Ethanol 70%	7023121	2
	Ethanol 70%	7024021	1
	Ethanol 70%	7024041	1
	Ethanol 70%	7024042	1
	Ethanol 70%	7024051	3
	Ethanol 70%	7024052	1
	Ethanol 70%	7024054	1
	Ethanol 70%	7024061	3
	Ethanol 70%	7024101	1
	Ethanol 70%	7024102	1
	Ethanol 70%	7024103	1
	Ethanol 70%	7025022	2
	Ethanol 70%	7025033	2
	Ethanol 70%	7025051	2
	Ethanol 70%	7025081	1
	Ethanol 70%	825A-02320	1
	Ethanol 70%	924I-02320	1
	Ethanol 70%	94/030724	1
	Ethanol 70%	Apotheke	1
	Ethanol 70%	RD240603-0001	1
	Ethanol 70%	RD240603-001	1
	Ethanol 70%	RD250514-0005	1
	Ethanol 70%	RD251103-0003	1
— (Retest)	Ethanol 70%	181009	1
A. Pflüger GmbH & Co. KG	Ethanol 70%	141127	1
A. Pflüger GmbH & Co. KG	Ethanol 70%	150209	1
A. Pflüger/Jenne	Ethanol 70%	131108	1
A. Pflüger/Phönix	Ethanol 70%	130607	1
A. Pflüger/Phönix	Ethanol 70%	130729	1
A. Plueger/ Noweda/ ...	Ethanol 70%	191121	2
A.Pflüger GmbH & Co....	Ethanol 70%	130514	1
A.Pflüger GmbH & Co....	Ethanol 70%	131011	1
A.Pflüger GmbH	Ethanol 70%	150730	1
A.Pflüger	Ethanol 70%	21111301	1
A.Pflüger/Noweda	Ethanol 70%	130116	1
Adler-Apotheke Rp 5	Ethanol 70%	1023A-02320	1
Adler-Apotheke Rp 5	Ethanol 70%	122A-02320	1
Adler-Apotheke Rp 5	Ethanol 70%	1422E-02320	1
Adler-Apotheke Rp 5	Ethanol 70%	2922E-02320	1
Adler-Apotheke Rp 5	Ethanol 70%	3021I-02320	1
AHC	Ethanol 70%		1
AHD	Ethanol 70%	170906	1
AHD	Ethanol 70%	200311	1
AHZ	Ethanol 70%	200415	1
AHZ	Ethanol 70%	FD200414-01A	1
AHZ	Ethanol 70%	FD200415-02B	1
AHZ	Ethanol 70%	FD200415-03A	1
AHZ	Ethanol 70%	FD200415-03B	1
AHZ	Ethanol 70%	FD200415-04A	1
AHZ	Ethanol 70%	FD200415-04B	1
AHZ	Ethanol 70%	Patient	1
Alkoholvertrieb Süd	Ethanol 70%	117332021	1
Alkoholvertrieb Süd	Ethanol 70%	121832022	1
Alkoholvertrieb Süd	Ethanol 70%	220121-162107	1
Alli	Ethanol 70%	230223	1

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Supplier	Substance	Batch	Spectra
Alliance	Ethanol 70%	1121223	2
Alte Apo Defektur	Ethanol 70%	1220E-02320	1
Alte Apo Defektur	Ethanol 70%	3019M-02320	1
Altenburger Destille...	Ethanol 70%		6
Anzag	Ethanol 70%	1121223	1
Anzag	Ethanol 70%	1160524	1
Anzag	Ethanol 70%	7027102	1
Anzag	Ethanol 70%	7028041	3
Anzag/ Otto Fischar ...	Ethanol 70%	7024051	1
Ap.am Bahnhof/Brüggemann	Ethanol 70%	1221Q-02320	1
Ap.am Bahnhof/Brüggemann	Ethanol 70%	1820A-02320	1
Ap.am Bahnhof/Brüggemann	Ethanol 70%	2720Q-02320	1
Ap.am Bahnhof/Brüggemann	Ethanol 70%	3020A-02320	1
Ap.am Bahnhof/Brüggemann	Ethanol 70%	5319A-02320	1
Apo	Ethanol 70%	523E-02320	1
apomix	Ethanol 70%	10A110522	2
apomix	Ethanol 70%	11A300320	2
apomix	Ethanol 70%	12A160718	1
apomix	Ethanol 70%	12A250116	1
apomix	Ethanol 70%	14A310718	1
apomix	Ethanol 70%	15A170215	1
apomix	Ethanol 70%	15a170918	1
apomix	Ethanol 70%	37A110416	1
apomix	Ethanol 70%	3A140119	1
apomix	Ethanol 70%	41A180515	1
apomix	Ethanol 70%	56a020715	1
apomix	Ethanol 70%	58A020715	1
apomix	Ethanol 70%	6A040213	1
apomix	Ethanol 70%	77A310815	1
Apotärze	Ethanol 70%	2015I-02320	1
Apotheke am Bahnhof ...	Ethanol 70%	4121I-02320	1
Apotheke am Bahnhof	Ethanol 70%	1023M-02320	1
Apotheke am Bahnhof	Ethanol 70%	2722I-02320	1
Apotheke am Bahnhof	Ethanol 70%	3622A-02320	2
Apotheke am Bahnhof/...	Ethanol 70%	3321A-02320	1
Apotheke am Grauturm	Ethanol 70%	320M-02320	1
Apotheke am Grauturm	Ethanol 70%	3920M-02320	3
Apotheke am Grauturm	Ethanol 70%	5221A-02320	1
Apotheke Eigenerstellung	Ethanol 70%	20221220S	1
Apotheke Gartenstadt	Ethanol 70%	1821M-02320	1
Apotheke Gartenstadt	Ethanol 70%	3921M-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	1720M-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	2020Q-03043	1
Apotheke Hornbach Zentrum	Ethanol 70%	2022Q-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	220720	1
Apotheke Hornbach Zentrum	Ethanol 70%	2721A-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	3120Q-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	4619A-02320	3
Apotheke Hornbach Zentrum	Ethanol 70%	4821A-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	5022E-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	5219Q-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	5320I-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	622A-02320	1
Apotheke im Forum	Ethanol 70%	150707	1
Apotheke im Forum	Ethanol 70%	300517	1
Apotheke im Medicus	Ethanol 70%	3321A-02320	1
Apotheke intern	Ethanol 70%	4921I-03043	1
Apotheke	Ethanol 70%		1
Apotheke	Ethanol 70%	190723003	1
apotheke	Ethanol 70%	290518h1	1

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Supplier	Substance	Batch	Spectra
Apotheke	Ethanol 70%	3621A-03043	1
Apotheke	Ethanol 70%	70105/51Dre	1
Apotheke	Ethanol 70%	70206/53Dre	1
Bahnhof Apotheke	Ethanol 70%	1218Q-03043	1
Bahnhof-Apothek/Bahn...	Ethanol 70%	3819A-03043	1
Bahnhofapotheke	Ethanol 70%	130320/6/20	1
Barlach Aptheke	Ethanol 70%	2015218	1
Barlach Aptheke	Ethanol 70%	3116M-03043	1
BBA	Ethanol 70%	4422E-02320	1
Behlen/Phönix	Ethanol 70%	1410T1300816	1
Belous	Ethanol 70%	4613E-02320	1
Berkel AHK	Ethanol 70%		1
Berkel AHK	Ethanol 70%	20042012397	1
Berkel AHK/HWA	Ethanol 70%	1410T31040613/70	1
Berliner Bär Apotheke	Ethanol 70%	2622I-02320	1
Berliner Bär Apotheke	Ethanol 70%	4321M-02320	1
Bombastus	Ethanol 70%	1061122	2
Bombastus	Ethanol 70%	150630	1
Brennerei Gauß	Ethanol 70%		1
Brennerei Gauß	Ethanol 70%	ML0G103/20	1
Brennerei Gauß	Ethanol 70%	ML0G505/2020	1
Brennerei Gauß	Ethanol 70%	ML0G604/2020	1
Brinn- Holtz	Ethanol 70%	1234-04/18	1
Brinn- Holtz	Ethanol 70%	1257-06/17	1
Buchner-Apotheke	Ethanol 70%	13221-02323	1
Caelo	Ethanol 70%		1
Caelo	Ethanol 70%	150730	1
Caelo	Ethanol 70%	171211	1
Caelo	Ethanol 70%	1715E-02320	1
Caelo	Ethanol 70%	1819A-02320	1
Caelo	Ethanol 70%	19151-02320	1
Caelo	Ethanol 70%	20140403	1
Caelo	Ethanol 70%	2614E-03043	1
Caelo	Ethanol 70%	3306	1
Caelo	Ethanol 70%	3A070918	1
Caelo	Ethanol 70%	46A120617	1
Caelo	Ethanol 70%	60307/50La	1
Caelo	Ethanol 70%	7022093	1
Caelo	Ethanol 70%	7023111	1
Caelo	Ethanol 70%	7025081	1
Caelo	Ethanol 70%	7028041	1
Caelo	Ethanol 70%	7028111	1
Caelo	Ethanol 70%	7028121	1
Caelo	Ethanol 70%	720318	1
Caelo	Ethanol 70%	814E-02320	1
Christina/Bioenergie...	Ethanol 70%	Eth70-08	1
Claudia Lange	Ethanol 70%	1234	1
Claudia Lange	Ethanol 70%	60919/50La	1
Claudia Lange	Ethanol 70%	61010/51La	1
Claudia Lange	Ethanol 70%	61107/50La	1
Defektur / Wolf-Apotheke	Ethanol 70%	60902/50Hk	1
Defektur 10.06.2013	Ethanol 70%	2013-06-10Defektur	1
Defektur 20.01.2014	Ethanol 70%	2014-01-20B	1
Defektur Apotheke	Ethanol 70%	1223A-07071	1
Defektur Apotheke	Ethanol 70%	819I-03043	1
Defektur- Apotheke	Ethanol 70%	622E-03043	1
Defektur	Ethanol 70%		9
Defektur	Ethanol 70%	1007210429	1
Defektur	Ethanol 70%	1020211104	1
Defektur	Ethanol 70%	1026211207	1

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Supplier	Substance	Batch	Spectra
Defektur	Ethanol 70%	122E-02320	1
Defektur	Ethanol 70%	1522E-02320	1
Defektur	Ethanol 70%	1716M-03043	1
Defektur	Ethanol 70%	1721M-02320	1
Defektur	Ethanol 70%	1LG20170224	1
Defektur	Ethanol 70%	1LG20171108	1
Defektur	Ethanol 70%	1MH20150818	1
Defektur	Ethanol 70%	200114Et0H70	1
Defektur	Ethanol 70%	2015Q-03043	1
Defektur	Ethanol 70%	2120E-02320	1
Defektur	Ethanol 70%	2220A-02320	1
Defektur	Ethanol 70%	23/14	1
Defektur	Ethanol 70%	2517A-07097	1
Defektur	Ethanol 70%	2617I-07097	1
Defektur	Ethanol 70%	2621M-02320	2
Defektur	Ethanol 70%	270613Et0H	1
Defektur	Ethanol 70%	2821Q-02320	1
Defektur	Ethanol 70%	3098	1
Defektur	Ethanol 70%	320E-02320	1
Defektur	Ethanol 70%	3219M-02320	1
Defektur	Ethanol 70%	321M-02320	1
Defektur	Ethanol 70%	3317M-03043	1
Defektur	Ethanol 70%	3420I-02320	1
Defektur	Ethanol 70%	3520E-02320	1
Defektur	Ethanol 70%	3820I-02320	1
Defektur	Ethanol 70%	3822Q-02320	1
Defektur	Ethanol 70%	4121M-02320	1
Defektur	Ethanol 70%	418I-07071	1
Defektur	Ethanol 70%	4319M-02320	1
DeFEKTUR	Ethanol 70%	4321I-02320	1
Defektur	Ethanol 70%	4520A-02320	2
Defektur	Ethanol 70%	4712M-02320	1
Defektur	Ethanol 70%	4714E-03043	1
Defektur	Ethanol 70%	5020Q-02320	1
Defektur	Ethanol 70%	50427/1La	1
Defektur	Ethanol 70%	50427/52Wlo	1
Defektur	Ethanol 70%	5117E-02320	1
Defektur	Ethanol 70%	5118I-02320	1
Defektur	Ethanol 70%	60209/51Hk	1
Defektur	Ethanol 70%	620Q-02320	1
Defektur	Ethanol 70%	71016/51Dre	1
Defektur	Ethanol 70%	719Q-02320	1
Defektur	Ethanol 70%	722Q-02320	1
Defektur	Ethanol 70%	80316/51Gie	1
Defektur	Ethanol 70%	80321/50Hk	1
Defektur	Ethanol 70%	80611/51Dre	1
Defektur	Ethanol 70%	93/250222	1
Defektur	Ethanol 70%	994201204	1
Defektur	Ethanol 70%	W150605	1
Defektur/Wolf Apotheke	Ethanol 70%	121Q-02320	1
Defektur/Wolf Apotheke	Ethanol 70%	2019E-07077	1
Defektur/Wolf Apotheke	Ethanol 70%	3321I-02320	1
Defektur/Wolf-Apotheke	Ethanol 70%	121M-02320	1
Defektur/Wolf-Apotheke	Ethanol 70%	1234567	2
Defektur/Wolf-Apotheke	Ethanol 70%	1621E-02320	2
Defektur/Wolf-Apotheke	Ethanol 70%	2321M-02320	1
Defektur/Wolf-Apotheke	Ethanol 70%	41211/51Hk	1
Defektur/Wolf-Apotheke	Ethanol 70%	4320I-02320	1
Defektur/Wolf-Apotheke	Ethanol 70%	50714/51Hk	1
Defektur/Wolf-Apotheke	Ethanol 70%	50714/53Hk	1

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Supplier	Substance	Batch	Spectra
Defektur/Wolf-Apotheke	Ethanol 70%	70227/52Dre	1
Die LindenApotheke /...	Ethanol 70%		1
Direktlieferung	Ethanol 70%		1
Doppeleiche Apotheke	Ethanol 70%	131227003	1
Doppeleiche Apotheke	Ethanol 70%	140303003	1
Doppeleiche Apotheke	Ethanol 70%	140630003	1
Doppeleiche Apotheke	Ethanol 70%	140927002	1
Doppeleiche Apotheke	Ethanol 70%	141029011	1
Doppeleiche Apotheke	Ethanol 70%	141208001	1
Doppeleiche Apotheke	Ethanol 70%	150114010	1
Doppeleiche Apotheke	Ethanol 70%	150126002	1
Doppeleiche Apotheke	Ethanol 70%	150219007	1
Doppeleiche Apotheke	Ethanol 70%	150504003	1
Doppeleiche Apotheke	Ethanol 70%	190219005	1
Doppeleiche Apotheke	Ethanol 70%	200806002	1
Doppeleiche Apotheke	Ethanol 70%	200901002	1
Doppeleiche Apotheke	Ethanol 70%	201021001	1
Doppeleiche Apotheke	Ethanol 70%	3013A-02320	1
Dr. Theis	Ethanol 70%	1030	1
Dreier	Ethanol 70%	201218	1
Dreikönigen Apotheke	Ethanol 70%	16049021	1
Dworzak	Ethanol 70%	220726-104957	1
Dworzak	Ethanol 70%	L10320	1
Eigen Löwen Apothke	Ethanol 70%	1722E-02320	1
eigen	Ethanol 70%		2
EIGEN	Ethanol 70%		1
Eigen	Ethanol 70%	1LG20180530	1
EIGEN	Ethanol 70%	2118I-03043	1
Eigen	Ethanol 70%	2419E-02320	1
Eigen	Ethanol 70%	3216E-03043	1
Eigen	Ethanol 70%	323-158	1
Eigen	Ethanol 70%	3319M-02320	1
EIGEN	Ethanol 70%	3419I-03043	1
Eigen	Ethanol 70%	4019Q-02320	3
Eigen	Ethanol 70%	4020A-02320	2
EIGEN	Ethanol 70%	4117I-03043	1
EIGEN	Ethanol 70%	4220E-02320	1
Eigen	Ethanol 70%	4318A-02320	2
Eigen	Ethanol 70%	4717E-03043	2
EIGEN	Ethanol 70%	4721E-02320	1
Eigen	Ethanol 70%	5016E-03043	1
EIGEN	Ethanol 70%	5218M-03043	1
Eigen	Ethanol 70%	616Q-03043	2
Eigen	Ethanol 70%	620A-02320	1
eigen	Ethanol 70%	622M-02320	1
Eigen	Ethanol 70%	eigen	1
Eigen	Ethanol 70%	Eigen	2
EIGEN	Ethanol 70%	EIGEN	1
Eigen/Defektur	Ethanol 70%	1116E-03043	1
Eigen/Defektur	Ethanol 70%	2516M-03043	1
Eigen/Defektur	Ethanol 70%	2716M-03043	1
Eigen/Defektur	Ethanol 70%	3416E-03043	1
Eigen/Deffektur	Ethanol 70%	1317A-02320	1
eigene Herstellung	Ethanol 70%	1712904-A	1
Eigene Herstellung	Ethanol 70%	2919E-02320	1
eigene Herstellung	Ethanol 70%	317E-02320	1
Eigene Herstellung	Ethanol 70%	3618I-02320	1
eigene Herstellung	Ethanol 70%	3620I-02320	1
eigene Herstellung	Ethanol 70%	3920A-02320	1
eigene Herstellung	Ethanol 70%	431140218	1

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Supplier	Substance	Batch	Spectra
eigene Herstellung	Ethanol 70%	4315Q-07016	1
eigene Herstellung	Ethanol 70%	4411312106	1
eigene Herstellung	Ethanol 70%	4819I-03043	1
eigene Herstellung	Ethanol 70%	6180115	1
Eigene Herstellung	Ethanol 70%	SP70140	1
Eigene Herstellung	Ethanol 70%	SPV7025	1
eigene herstellung	Ethanol 70%	SPV7026	1
Eigene Herstellung	Ethanol 70%	SPV7029	1
eigene	Ethanol 70%	1018E-02320	1
eigene	Ethanol 70%	219I-02320	1
eigene	Ethanol 70%	2619E-02320	1
Eigene	Ethanol 70%	621E-02320	1
Eigenherstellung Löw...	Ethanol 70%	1521E-02320	1
Eigenherstellung Löw...	Ethanol 70%	5220E-02320	1
Eigenherstellung-Biozid	Ethanol 70%	FP200430-04	1
Eigenherstellung	Ethanol 70%		2
Eigenherstellung	Ethanol 70%	1313I-02320	1
Eigenherstellung	Ethanol 70%	14032019-01	1
Eigenherstellung	Ethanol 70%	1515I-02320	1
Eigenherstellung	Ethanol 70%	170828001	1
Eigenherstellung	Ethanol 70%	1722Q-02320	1
eigenherstellung	Ethanol 70%	1819M-02320	2
Eigenherstellung	Ethanol 70%	1822A-03043	1
Eigenherstellung	Ethanol 70%	1823	1
Eigenherstellung	Ethanol 70%	19129501	1
Eigenherstellung	Ethanol 70%	200715-01	1
Eigenherstellung	Ethanol 70%	2015E-02320	1
Eigenherstellung	Ethanol 70%	20210816A	1
Eigenherstellung	Ethanol 70%	2105912	1
Eigenherstellung	Ethanol 70%	2124	1
Eigenherstellung	Ethanol 70%	2216A-02320	1
Eigenherstellung	Ethanol 70%	2314I-02320	1
Eigenherstellung	Ethanol 70%	2409219	1
Eigenherstellung	Ethanol 70%	2613I-03043	1
Eigenherstellung	Ethanol 70%	2753	1
Eigenherstellung	Ethanol 70%	321Q-02320	1
Eigenherstellung	Ethanol 70%	3413I-02320	1
Eigenherstellung	Ethanol 70%	3416E-02320	1
Eigenherstellung	Ethanol 70%	3521E-02320	1
eigenherstellung	Ethanol 70%	3818Q-02320	1
Eigenherstellung	Ethanol 70%	4215I-02320	1
Eigenherstellung	Ethanol 70%	4414A-02320	1
Eigenherstellung	Ethanol 70%	4513I-02320	1
Eigenherstellung	Ethanol 70%	4615	1
Eigenherstellung	Ethanol 70%	4715M	1
Eigenherstellung	Ethanol 70%	4733	1
Eigenherstellung	Ethanol 70%	5131213	1
Eigenherstellung	Ethanol 70%	517Q-02320	1
Eigenherstellung	Ethanol 70%	5214A-02320	1
Eigenherstellung	Ethanol 70%	5318A-02320	1
Eigenherstellung	Ethanol 70%	616Q-02320	1
Eigenherstellung	Ethanol 70%	Eigenherstellung	1
Eigenproduktion	Ethanol 70%	1217Q-02320	1
Eigenproduktion	Ethanol 70%	714Q-02320	1
Engel-Apotheke	Ethanol 70%	2319A-07016	1
Engel/Engel	Ethanol 70%	39-28715	1
Euro OTC	Ethanol 70%	15A170918	1
Euro OTC	Ethanol 70%	170116	1
Euro OTC	Ethanol 70%	220713	1
Euro OTC	Ethanol 70%	7028031	2

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Supplier	Substance	Batch	Spectra
Euro OTC	Ethanol 70%	77A110917	1
Fagron	Ethanol 70%	40929/52La	1
Fagron	Ethanol 70%	7027102	1
Fagron	Ethanol 70%	Probemessung	1
Falken-Apotheke	Ethanol 70%	8221-03043	1
Fiebig	Ethanol 70%	7029051	1
Fischar / Alliance ...	Ethanol 70%	7026051	1
Fischar / Alliance ...	Ethanol 70%	7028102	1
Fischar / Alliance ...	Ethanol 70%	7029041	1
Fischar / A	Ethanol 70%	7022081	3
Fischar / Anzag	Ethanol 70%	7023091	1
Fischar / Noweda	Ethanol 70%	7023111	1
Fischar / Noweda	Ethanol 70%	7024021	1
Fischar / Sanacorp	Ethanol 70%	7023091	1
Fischar GmbH	Ethanol 70%	7028062	1
Fischar, Gehe	Ethanol 70%	7022031	1
Fischar	Ethanol 70%		1
Fischar	Ethanol 70%	27031501	1
fischar	Ethanol 70%	7020012	1
fischar	Ethanol 70%	7020032	1
Fischar	Ethanol 70%	7020046	1
fischar	Ethanol 70%	7021101	1
Fischar	Ethanol 70%	7022022	1
Fischar	Ethanol 70%	7022051	1
Fischar	Ethanol 70%	7022093	1
Fischar	Ethanol 70%	7024051	1
Fischar	Ethanol 70%	7025082	1
Fischar	Ethanol 70%	7028011	1
Fischar	Ethanol 70%	7028031	1
Fischar	Ethanol 70%	7028041	1
Fischar	Ethanol 70%	7028062	1
Fischar	Ethanol 70%	7028081	1
Fischar	Ethanol 70%	7029082	3
Fischar	Ethanol 70%	7029101	1
Fischar/ Gehe	Ethanol 70%	7020101	1
Fischar/ Gehe	Ethanol 70%	7020102	1
Fischar/ Gehe	Ethanol 70%	7021051	1
Fischar/ Gehe	Ethanol 70%	7022061	1
Fischar/ Phoenix/ 25...	Ethanol 70%	7028121	1
Fischar/ Phoenix/ 29...	Ethanol 70%	7029031	1
Fischar/ Sanacorp	Ethanol 70%	7021081	1
Fischar/Gehe	Ethanol 70%	7022102	1
Fischar/Novatis	Ethanol 70%	701004810049	1
Fischar/Novatis	Ethanol 70%	7020113	1
Fischar/Noweda	Ethanol 70%	702004b	1
Fischar/Noweda	Ethanol 70%	7022023	1
Fischar/Phoenix	Ethanol 70%	7028081	1
Fischar/Phoenix	Ethanol 70%	7029102	1
Fischar/Phönix	Ethanol 70%	7020046	1
Fischar/Phönix	Ethanol 70%	7021092	1
Fischar/Phönix	Ethanol 70%	7026031	1
Fischar/Phönix	Ethanol 70%	7026092	1
Fischar/Phönix	Ethanol 70%	7026111	1
Fischar/Phönix	Ethanol 70%	7027031	2
fischar/Phönix	Ethanol 70%	7027032	1
Fischar/Phönix	Ethanol 70%	7028102	1
Fischar/Sanacorp	Ethanol 70%	7027102	1
Fischar/Sanacorp	Ethanol 70%	7028031	1
Fischar/Sanacorp	Ethanol 70%	7028062	1
Fischar/Sanacorp	Ethanol 70%	7028081	1

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Supplier	Substance	Batch	Spectra
Fischer	Ethanol 70%	7028111	1
Fischer/Noweda	Ethanol 70%	702003F	1
Fischer/sanacorp	Ethanol 70%	702003G	1
FischerGehe	Ethanol 70%	702003H	1
fishar	Ethanol 70%	7028111	1
frischhergestellt	Ethanol 70%		2
Gehe 27.2.14	Ethanol 70%	140121	1
Gehe-Kremer	Ethanol 70%	140307	1
Gehe-Kremer	Ethanol 70%	150209	1
GEHE	Ethanol 70%	1191224	1
GEHE	Ethanol 70%	180828	1
Gehe	Ethanol 70%	3818Q-02320	1
Gehe	Ethanol 70%	7022093	2
Gehe	Ethanol 70%	7023022	1
Gehe	Ethanol 70%	7023101	1
Gehe	Ethanol 70%	7024044	1
Gehe	Ethanol 70%	7024054	1
GEHE/Otto Fischar GmbH	Ethanol 70%	7020049	1
Gehe/Pflüger	Ethanol 70%	1204021712	1
Gehe/Pflüger	Ethanol 70%	160909	2
Gehe/Pflüger	Ethanol 70%	170208	1
Gehe/Pflüger	Ethanol 70%	170308	1
Gehe/Pflüger	Ethanol 70%	170419	2
Gehe/Pflüger	Ethanol 70%	180928	1
Gehe/PKH	Ethanol 70%	28A300420	1
Geibo/Teopharm 4.2.22	Ethanol 70%	21001T	1
Gersprenz Apo	Ethanol 70%	3519A-02320	1
Goethe Apotheke	Ethanol 70%	RD201026-0002	1
Goetheapotheke	Ethanol 70%	3820E-03043	1
Gutenberg-Apotheke	Ethanol 70%	130502003	1
Gutenberg-Apotheke	Ethanol 70%	1813M-02320	1
Gutenberg-Apotheke	Ethanol 70%	3412I-03043	1
Heck/Wittich	Ethanol 70%	2113N-02320	1
Hedinger/Phoe	Ethanol 70%	170308	2
Hermes	Ethanol 70%	3720I	1
Hetterich - Teofarma...	Ethanol 70%	145501/R	2
Hetterich - Teofarma...	Ethanol 70%	145601	3
Hetterich (FAM)	Ethanol 70%	145003	1
Hetterich/ Noweda	Ethanol 70%	145703	1
Hetterich/ Noweda	Ethanol 70%	145802	1
Hetterich/ Noweda	Ethanol 70%	1801T	1
Hetterich/ Sanacorp	Ethanol 70%	145703	1
Hetterich/AEP	Ethanol 70%	145802	1
Hetterich/AllianceH.	Ethanol 70%	145703	2
Hetterich/Ebert	Ethanol 70%	145401	2
Hettrich/FAM	Ethanol 70%	145802	2
Hirsch Apo	Ethanol 70%	923I-02320	1
Hirsch	Ethanol 70%	4413I-02320	1
Hirsch	Ethanol 70%	714E-02320	1
HirschApotheke	Ethanol 70%	1015I-02320	1
HirschApotheke	Ethanol 70%	2315I-02320	1
HirschApotheke	Ethanol 70%	4614A-02320	1
Hoffmann / Bahnhof A...	Ethanol 70%	3919A-02320	1
Hoffmann & Sommer Gm...	Ethanol 70%	580916	1
Hoffmann & Sommer Gm...	Ethanol 70%	650917	1
Hoffmann & Sommer	Ethanol 70%	750718	1
Hoffmann	Ethanol 70%	781218	1
Hoffmann&Sommer	Ethanol 70%	1010520	5
Hoffmann&Sommer	Ethanol 70%	1020520	11
Hoffmann&Sommer	Ethanol 70%	1030620	9

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Supplier	Substance	Batch	Spectra
Hoffmann&Sommer	Ethanol 70%	1050622	8
Hoffmann&Sommer	Ethanol 70%	1070123	7
Hoffmann&Sommer	Ethanol 70%	1090423	7
Hoffmann&Sommer	Ethanol 70%	52023	1
Hoffmanns/Anzag	Ethanol 70%	520116	1
Hofman und Sommer Gm...	Ethanol 70%	580916	1
Hofmann / Phönix	Ethanol 70%	840819	1
Hofmann /Phoenix	Ethanol 70%	900320	1
Hofmann & Sommer Gmb...	Ethanol 70%	1020520	1
Hofmann & Sommer Gmb...	Ethanol 70%	1061122	1
Hofmann & Sommer	Ethanol 70%	1010520	1
Hofmann & Sommer	Ethanol 70%	691217	1
Hofmann et Sommer	Ethanol 70%	1000520	1
Hofmann Sommer	Ethanol 70%	970420	1
Hofmann u. Sommer	Ethanol 70%	720318	1
Hofmann und Sommer	Ethanol 70%	980520	1
Hofmann	Ethanol 70%	320713	1
Hofmann's	Ethanol 70%	940420	1
Hofmanns / Noweda	Ethanol 70%	820419	1
Hofmann&Sommer GmbH ...	Ethanol 70%	1010520	2
Hofmann&Sommer GmbH ...	Ethanol 70%	940420	7
Hofmann&Sommer GmbH ...	Ethanol 70%	950420	9
Hofmann&Sommer	Ethanol 70%	940420	1
Hofmann&Sommer/Sanacorp	Ethanol 70%	781218	1
Hofmanns/AHD	Ethanol 70%	1010520	2
hofmanns/noweda	Ethanol 70%	890320	1
hofmanns/noweda	Ethanol 70%	960420	1
Hohe-Wart-Apotheke	Ethanol 70%	23072013/1	1
Homöopathisches Labo...	Ethanol 70%	200327	1
Hubertus Apotheke	Ethanol 70%	261113	1
Iipse	Ethanol 70%	3922M-02320	1
Kastner (eigen)	Ethanol 70%	1215E-02320	1
Kastner (eigen)	Ethanol 70%	3114E-03043	1
Kehr	Ethanol 70%	230111	1
Kehr/Pflüger	Ethanol 70%	200302	1
Kehr/Pflüger	Ethanol 70%	20031	1
Kehr/Pflüger	Ethanol 70%	200427	1
Kemer Phönix	Ethanol 70%	130628	1
Klenk	Ethanol 70%	150730	1
Kremer / Hageda	Ethanol 70%	161017	1
Kremer GmbH / Gehe	Ethanol 70%	160909	1
Kremer GmbH / Noweda	Ethanol 70%	140627	1
Kremer GmbH / Noweda	Ethanol 70%	141127	2
Kremer GmbH & Co. KG	Ethanol 70%	180828	2
Kremer GmbH & Co.KG	Ethanol 70%	140902	2
Kremer GmbH & Co.KG	Ethanol 70%	150602	1
Kremer GmbH &Co. KG	Ethanol 70%	160215	1
Kremer GmbH &Co. KG	Ethanol 70%	161017	1
Kremer GmbH &Co. KG	Ethanol 70%	170116	2
Kremer GmbH &Co. KG	Ethanol 70%	170208	1
Kremer GmbH &Co. KG	Ethanol 70%	170619	4
Kremer GmbH Wupperta...	Ethanol 70%	130729	1
Kremer GmbH	Ethanol 70%	160512	1
Kremer GmbH	Ethanol 70%	170906	1
Kremer GmbH	Ethanol 70%	181206	1
kremer gmbh	Ethanol 70%	23081605	1
Kremer GmbH	Ethanol 70%	unbekannt	1
Kremer GmbH/Noweda	Ethanol 70%	181115	1
Kremer GmbH/Phönix	Ethanol 70%	150327	1
Kremer	Ethanol 70%	130206	1

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Supplier	Substance	Batch	Spectra
Kremer	Ethanol 70%	141027	1
Kremer	Ethanol 70%	160414	1
Kremer	Ethanol 70%	160711	1
Kremer	Ethanol 70%	160909	1
Kremer	Ethanol 70%	161017	1
Kremer	Ethanol 70%	170208	1
Kremer	Ethanol 70%	170308	1
Kremer	Ethanol 70%	170619	1
Kremer	Ethanol 70%	180404	1
Kremer	Ethanol 70%	180525	1
Kremer	Ethanol 70%	180828	2
Kremer	Ethanol 70%	181206	1
Kremer/Alliance Heal...	Ethanol 70%	171025	1
Kremer/Gehe	Ethanol 70%	130116	1
Kremer/Gehe	Ethanol 70%	140121	1
Kremer/Gehe	Ethanol 70%	160414	2
Kremer/hageda	Ethanol 70%	16025	1
Kremer/Noweda	Ethanol 70%	131011	1
Kremer/Noweda	Ethanol 70%	170906	1
Kremer/Phoenix	Ethanol 70%	150730	1
Kremer/Phönix	Ethanol 70%	141127	1
Kremer/Phönix	Ethanol 70%	150327	1
Kremer/Phönix	Ethanol 70%	151123	1
Kremer/Phönix	Ethanol 70%	180404	1
Kremer/Phönix	Ethanol 70%	180928	1
Kremer/Phönix	Ethanol 70%	190321	1
KremperGmbH & Co. KG	Ethanol 70%	140507	1
Kreuzäcker Apotheke	Ethanol 70%	322E-02320	1
Kreuzäcker Apotheke	Ethanol 70%	3619A-02320	1
Kreuzäcker Apotheke	Ethanol 70%	619I-02320	1
Kreuzäcker Apotheke	Ethanol 70%	K211021Ri	1
kruppa	Ethanol 70%	1216H4	1
Kruppa	Ethanol 70%	418H2	1
kruppa	Ethanol 70%	617H4	1
Kruppa	Ethanol 70%	818H2	1
Lamotte/AHCA	Ethanol 70%	6007153001	1
Lamotte/AHCA	Ethanol 70%	6010634001	4
Libellen Apotheke	Ethanol 70%	1515Q-02320	1
Löwen-Apotheke	Ethanol 70%	219Q-03043	1
Martinus-Apotheke De...	Ethanol 70%	E-090520-1D	1
Martinus-Apotheke De...	Ethanol 70%	E-160321-1D	1
Martinus-Apotheke	Ethanol 70%	A-061213-3D	1
Martinus-Apotheke	Ethanol 70%	A-311013-1D	1
Martinus-Apotheke	Ethanol 70%	E-020314-1D	1
Martinus-Apotheke	Ethanol 70%	E-021116-1D	1
Martinus-Apotheke	Ethanol 70%	E-050515-1D	1
Martinus-Apotheke	Ethanol 70%	E-080514-1D	1
Martinus-Apotheke	Ethanol 70%	E-100114-1D	1
Martinus-Apotheke	Ethanol 70%	E-110716-1D	1
Martinus-Apotheke	Ethanol 70%	E-121214-1D	1
Martinus-Apotheke	Ethanol 70%	E-140119-1D	1
Martinus-Apotheke	Ethanol 70%	E-180118-1D	1
Martinus-Apotheke	Ethanol 70%	E-180714-1D	1
Medicon Apotheke Defektur	Ethanol 70%	4122A-02320	1
Met/ Noweda	Ethanol 70%	3815M-03043	1
n.a.	Ethanol 70%	1707918-a	1
Nachprüfung	Ethanol 70%		1
Noweda	Ethanol 70%	1191224	1
Noweda	Ethanol 70%	120420	1
Noweda	Ethanol 70%	145703	1

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Supplier	Substance	Batch	Spectra
Noweda	Ethanol 70%	145804	1
Noweda	Ethanol 70%	190717	4
Noweda	Ethanol 70%	190815	2
Noweda	Ethanol 70%	200330	1
noweda	Ethanol 70%	7023101	1
Noweda	Ethanol 70%	7024011	1
Noweda/Hoffmann&Sommer	Ethanol 70%	1061122	3
Noweda/Hofmanns	Ethanol 70%	860120	1
Noweda/Kremer GmbH	Ethanol 70%	181115	1
Noweda/KremerGmbH	Ethanol 70%	130821	1
Noweda/Pflüger	Ethanol 70%	190606	1
Noweda/Pflüger	Ethanol 70%	200330	1
O:Fischar/Phönix	Ethanol 70%	7027032	1
Otto Fischar GmbH & ...	Ethanol 70%	702003D	1
OTTO FISCHAR GmbH & ...	Ethanol 70%	7021083	3
OTTO FISCHAR GmbH & ...	Ethanol 70%	7022021	1
Otto Fischar GmbH & ...	Ethanol 70%	7024021	1
Otto Fischar GmbH & ...	Ethanol 70%	7025031	2
Otto Fischar GmbH & ...	Ethanol 70%	7028041	1
Otto Fischar GmbH & ...	Ethanol 70%	7024071	1
Otto Fischar GmbH & Co KG	Ethanol 70%	7020043	1
Otto Fischar GmbH	Ethanol 70%	702003N	1
Otto Fischar GmbH	Ethanol 70%	7022072	1
Otto Fischar GmbH/ Amzag	Ethanol 70%	7024091	1
Otto Fischar GmbH/ Noweda	Ethanol 70%	7021092	1
Otto Fischar, Gehe	Ethanol 70%	7029041	1
Otto Fischar	Ethanol 70%	702004A	1
Otto Fischar	Ethanol 70%	7023111	1
Otto Fischar	Ethanol 70%	7028121	1
Otto Fischar/ Anzag	Ethanol 70%	7029021	1
Otto Fischer / Noweda	Ethanol 70%	7025031	1
Otto Fischer /Phönix	Ethanol 70%	702004B	1
Otto Fischer GmbH & ...	Ethanol 70%	7029121	1
Otto Fischer GmbH	Ethanol 70%	7020031	1
Otto Fischer GmbH	Ethanol 70%	7020045	2
Otto Fischer GmbH/Sa...	Ethanol 70%	7021092	1
Otto Fischer GmbH&Co...	Ethanol 70%	7028091	1
Otto Fischer/ Noweda	Ethanol 70%	7029051	1
otto Fischer/Noweda	Ethanol 70%	7024121	1
Otto/Fischer	Ethanol 70%	1029051	1
Pflüger 13.03.2020 E...	Ethanol 70%	200303	1
Pflüger GmbH / Gehe	Ethanol 70%	180404	1
Pflüger GmbH / Noweda	Ethanol 70%	190717	1
Pflüger GmbH / Noweda	Ethanol 70%	200319	1
Pflüger GmbH & Co.KG	Ethanol 70%	170116	1
Pflüger GmbH	Ethanol 70%	191121	2
Pflüger	Ethanol 70%	130607	1
Pflüger	Ethanol 70%	131108	2
Pflüger	Ethanol 70%	141027	1
Pflüger	Ethanol 70%	170906	1
Pflüger	Ethanol 70%	171025	1
Pflüger	Ethanol 70%	180308	1
Pflüger	Ethanol 70%	190430	3
Pflüger	Ethanol 70%	190606	1
Pflüger	Ethanol 70%	190717	1
Pflüger	Ethanol 70%	200302	1
Pflüger	Ethanol 70%	200310	1
Pflüger	Ethanol 70%	200311	2
Pflüger	Ethanol 70%	200313	1
PFLÜGER	Ethanol 70%	200321	1

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Supplier	Substance	Batch	Spectra
Pflüger/ Noweda	Ethanol 70%	180404	1
Pflüger/AHC	Ethanol 70%	200303	1
Pflüger/Alliance Hea...	Ethanol 70%	200407	1
Pflüger/Alliance Hea...	Ethanol 70%	200410	1
Pflüger/Alliance Hea...	Ethanol 70%	221020	2
Pflüger/Gehe	Ethanol 70%	170619	1
Pflüger/Gehe	Ethanol 70%	181115	1
Pflüger/Gehe	Ethanol 70%	200313	1
Pflüger/Jenne	Ethanol 70%	200303	1
Pflüger/Kehr	Ethanol 70%	190430	1
Pflüger/Kehr	Ethanol 70%	200316	1
Pflüger/kehr	Ethanol 70%	200327	1
Pflüger/Kehr	Ethanol 70%	200411	1
Pflüger/Kehr	Ethanol 70%	230111	1
Pflüger/Noweda	Ethanol 70%	190815	1
Pflüger/Noweda	Ethanol 70%	200319	2
Pflüger/Noweda	Ethanol 70%	200409	1
Pflüger/Phönix	Ethanol 70%	190430	1
Pflüger/Phönix	Ethanol 70%	200319	1
Phoenix	Ethanol 70%	170116	1
Phoenix	Ethanol 70%	170619	1
Phoenix	Ethanol 70%	170717	2
phoenix	Ethanol 70%	170906	1
Phoenix	Ethanol 70%	7025012	1
Phoenix	Ethanol 70%	7027032	1
Phoenix	Ethanol 70%	7027103	1
Phoenix	Ethanol 70%	7029082	1
Phönix	Ethanol 70%	1070123	2
PHÖNIX	Ethanol 70%	171025	1
PHÖNIX	Ethanol 70%	171211	1
Phönix	Ethanol 70%	351213	1
Phönix/Kremer	Ethanol 70%	160711	1
Phönix/Kremer	Ethanol 70%	180525	1
Phönix/Otto Fischar	Ethanol 70%	7029082	1
PKH GmbH	Ethanol 70%	4A070518	1
PKH	Ethanol 70%	33A290620	1
Plüger/Anzag	Ethanol 70%	32016	1
Post Apotheke	Ethanol 70%	323-160	1
Post Apotheke	Ethanol 70%	323-161	1
Post-Apotheke 15.01.2014	Ethanol 70%	15012044	1
Post-Apotheke	Ethanol 70%	1414A-02320	1
Purren Apotheke	Ethanol 70%	17043	1
Rats-Apotheke	Ethanol 70%	4022N-02320	1
Regenbogen Apotheke	Ethanol 70%	1219E-03043	1
Regenbogen Apotheke	Ethanol 70%	21119A-03043	1
Regenbogen Apotheke	Ethanol 70%	3120Q-03043	1
Regenbogen Apotheke	Ethanol 70%	4721A-02320	1
Regenbogen Apotheke	Ethanol 70%	4818A-03043	1
Regenbogen Apotheke	Ethanol 70%	5119E-03043	1
Rezeptur Apotheke	Ethanol 70%	2016Q-03043	1
Rezeptur Apotheke	Ethanol 70%	917Q-03043	1
Rezeptur	Ethanol 70%	4215Q-03043	1
Rezeptur	Ethanol 70%	622I03043	1
Roland-Apotheke	Ethanol 70%	2620E-03043	1
Roland-Apotheke	Ethanol 70%	3519M-03043	1
Römer-Apotheke	Ethanol 70%	4314A-03043	1
Rondell Apotheke	Ethanol 70%	1814Q-07145	1
Rondell Apotheke	Ethanol 70%	26151-07145	1
Rondell Apotheke	Ethanol 70%	2616M-02320	1
Rondell Apotheke	Ethanol 70%	3414M-02320	1

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Supplier	Substance	Batch	Spectra
Rondell Apotheke	Ethanol 70%	3414M-07145	1
Rondell Apotheke	Ethanol 70%	4015A-03043	1
Rondell Apotheke	Ethanol 70%	415M-03043	1
Rondell Apotheke	Ethanol 70%	416M-02320	1
Rondell Apotheke	Ethanol 70%	615E-02320	1
Rondell Apotheke	Ethanol 70%	615E-07145	1
Rondell	Ethanol 70%	1715E-07145	1
Rosen Apotheke	Ethanol 70%	1-040821	1
Rosen Apotheke	Ethanol 70%	1317A-07095	1
Rosen-Apotheke	Ethanol 70%	1-030320	1
Rosen-Apotheke	Ethanol 70%	1-100321	1
Rosen-Apotheke	Ethanol 70%	1-171121	2
Rosen-Apotheke	Ethanol 70%	2-080922	1
Rosen-Apotheke	Ethanol 70%	2-120320	1
Rosen-Apotheke	Ethanol 70%	2-190721	1
Rosen-Apotheke	Ethanol 70%	3-081021	1
Rosen-Apotheke	Ethanol 70%	4-260520	1
Rosen-Apotheke	Ethanol 70%	5-270720	1
Rosen-Apotheke	Ethanol 70%	6-061120	1
Rosen-Apotheke	Ethanol 70%	7-291220	1
Rosenapotheke	Ethanol 70%	2317E-07095	1
Sanacorp	Ethanol 70%	1061122	1
Sanacorp	Ethanol 70%	1110723	2
Sanacorp	Ethanol 70%	1121223	1
Sanacorp	Ethanol 70%	130124	1
Sanacorp	Ethanol 70%	702003D	1
Sanacorp	Ethanol 70%	7020075	1
Sanacorp	Ethanol 70%	7028081	3
Sanacorp/Pflüger	Ethanol 70%	170906	1
selbst hergestellt	Ethanol 70%	1MH20151222	1
selbst hergestellt	Ethanol 70%	1MH20160304	1
selbst hergestellt	Ethanol 70%	1MH20160721	1
selbst hergestellt	Ethanol 70%	1MH20160921	1
selbst hergestellt	Ethanol 70%	1MH20161011	1
selbst hergestellt	Ethanol 70%	1MH20170710	1
sittig	Ethanol 70%	310316	1
Sittig	Ethanol 70%	90623	1
SonnenApo	Ethanol 70%	2613I-02230	1
SonnenApo	Ethanol 70%	5122E-03043	1
St. Martin Apotheke ...	Ethanol 70%	2822I-02320	2
St. Martin Apotheke ...	Ethanol 70%	4322I-02320	1
St. Martin Apotheke	Ethanol 70%	1020M-02320	1
St. Martin Apotheke	Ethanol 70%	1022A-02320	1
St. Martin Apotheke	Ethanol 70%	2321A-02320	1
St. Martin Apotheke	Ethanol 70%	320M-02320	1
St. Martin Apotheke	Ethanol 70%	821E-02320	1
Stadt-Apo	Ethanol 70%	5018A-03043	2
Stern-Defektur	Ethanol 70%	130705003	1
Stiftsapotheke	Ethanol 70%	13052016	1
Stiftsapotheke	Ethanol 70%	150420005	1
Teofarma R.r.l.	Ethanol 70%	20002T	1
Theiss	Ethanol 70%	2040	1
Töste Apotheke	Ethanol 70%	1119A-03043	1
Töste Apotheke	Ethanol 70%	1321A-07134	1
Töste Apotheke	Ethanol 70%	1921E-03403	1
Töste Apotheke	Ethanol 70%	2122E-02320	1
Töste Apotheke	Ethanol 70%	2520A-03043	1
Töste Apotheke	Ethanol 70%	2919A-03043	1
Töste Apotheke	Ethanol 70%	3021A-02320	1
Töste Apotheke	Ethanol 70%	319E-03043	1

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Supplier	Substance	Batch	Spectra
Töste Apotheke	Ethanol 70%	3612M-02320	1
Töste Apotheke	Ethanol 70%	4021A-02320	1
Töste Apotheke	Ethanol 70%	4819A-03043	1
Töste Apotheke	Ethanol 70%	922A-02320	1
Viehstrich-Apotheke	Ethanol 70%	3219E-03043	1
Vita Apotheke	Ethanol 70%	190531006	1
VitaFit	Ethanol 70%	2020-04-17	2
Vital	Ethanol 70%	50821	1
VWR Chemicals	Ethanol 70%	20b254009	1
VWR Chemicals	Ethanol 70%	20B254009	1
Wolf Apotheke/Defektur	Ethanol 70%	70627/52Hk	1
Wolf Apotheke/Defektur	Ethanol 70%	71208/50Gie	1
Wolf-Apotheke / Defektur	Ethanol 70%	40722/51Hk	1
Wolf-Apotheke / Defektur	Ethanol 70%	41125/52Hk	1
Wolf-Apotheke / Defektur	Ethanol 70%	51019/51Wlo	1
Wolf-Apotheke / Defektur	Ethanol 70%	70404/53Hk	1
Wolf-Apotheke / Defektur	Ethanol 70%	Bulk	1
Wolf-Apotheke-Defektur	Ethanol 70%	70818/50Hk	1
Wolf-Apotheke	Ethanol 70%	40331/52La	1
Wolf-Apotheke	Ethanol 70%	4321E-02320	1

- 19 727 spectra from 1539 *Apo-Ident* customers from a total of 5629 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ethanol 70%* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ethanol 70%* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	240	0	27 694
Type B	0	160	0	30 770
Type C	0	1035	16	19 727

The substance/substance group *Ethanol 70%* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.0582 %)	98.4776 % (> 98.1922 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30779	30779	0.00	100.15
31055	31055	0.00	82.46
34101	34101	0.00	94.68
34274	34274	0.00	81.51
38759	38759	0.00	75.37

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Fat ointments**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30881-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Fat ointments; Asche Basis[®] fat ointment; Cottonwood ointment; Deumavan[®] protection ointment neutral; Marjoram ointment; Neribas[®] fat ointment; Protegin[®] XN; Unguentum majoranae; Unguentum Populi

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Fat ointments	27	31	276

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fat ointments* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
White paraffin oil	11.29	—
Wax ointment	25.93	—
Lygal [®] ointment base	32.15	—
Stomahesive [®] adhesive paste	66.22	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Fat ointments*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Chiesi	Asche Basis [®] fat ointment	23014A	31013	40	not required
Chiesi	Asche Basis [®] fat ointment	41017A	31858	60	not required
Chiesi	Asche Basis [®] fat ointment	53021A	33634	40	not required
Chiesi	Asche Basis [®] fat ointment	02004A	35471	40	not required
Caelo	Cottonwood ointment	161175	32473	40	20160607*
Caelo	Cottonwood ointment	170572	33130	40	20170307*
Caelo	Cottonwood ointment	170573	33131	40	20170308*
Caelo	Cottonwood ointment	191253	34783	40	20190529*
Caelo	Cottonwood ointment	20001373	34966	40	20200513*
Caelo	Cottonwood ointment	20000881	34967	40	20200325*
Caelo	Cottonwood ointment	22002922	36671	40	20221121*
Kaymogyn GmbH	Deumavan [®] protection oint...	41920120	35069	40	not required
Kaymogyn GmbH	Deumavan [®] protection oint...	13781119	35071	40	not required
Kaymogyn GmbH	Deumavan [®] protection oint...	31660422	36744	40	not required
Caelo	Marjoram ointment	12123001	30881	40	not required
Caelo	Marjoram ointment	14089901	31443	40	not required
Caelo	Marjoram ointment	20000281	34963	40	20200207*
Caelo	Marjoram ointment	21000565	35346	40	20210326*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Marjoram ointment	22000091	36144	40	20220302*
Henry Lamotte	Marjoram ointment	5322500	30926	40	not required
Jenapharm	Neribas [®] fat ointment	32032C	31489	40	not required
Jenapharm	Neribas [®] fat ointment	YY00K7C	31872	60	not required
Jenapharm	Neribas [®] fat ointment	YY01TF2	33986	40	not required
Caelo	Protegin [®] XN	13081901	31112	40	not required
Caelo	Protegin [®] XN	13344402	31475	40	not required
Caelo	Protegin [®] XN	17258703	33921	40	not required
Caelo	Protegin [®] XN	24001198	38641	40	20240514*

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1120 spectra of 27 reference samples from the substance/substance group *Fat ointments*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 27 different batches.
- 26 814 spectra from a total of 573 batches from further 138 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 1150 spectra of 33 reference samples from the substance/substance group *Fat ointments*.
- Among them are spectra of independent samples from 31 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Chiesi	Asche Basis [®] fat ointment	24010A	37420	40
Caelo	Cottonwood ointment	170534	33162	40
Caelo	Cottonwood ointment	170574	33163	40
Caelo	Cottonwood ointment	180826	34186	40
Caelo	Cottonwood ointment	180828	34187	40

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

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cottonwood ointment	181888	34256	40
Caelo	Cottonwood ointment	21000483	35336	40
Caelo	Cottonwood ointment	22000087	36077	40
Caelo	Cottonwood ointment	22000088	36078	40
Caelo	Cottonwood ointment	22000089	36079	10
Caelo	Cottonwood ointment	22000090	36080	10
Caelo	Cottonwood ointment	22002923	36672	10
Caelo	Cottonwood ointment	22002924	36673	10
Caelo	Cottonwood ointment	22003582	36674	10
Caelo	Cottonwood ointment	23000816	37535	40
Caelo	Cottonwood ointment	23000817	37536	10
Caelo	Cottonwood ointment	23000818	37537	10
Kaymogyn GmbH	Deumavan [®] protection oint...	62170320	35070	40
Caelo	Marjoram ointment	153533	31990	60
Caelo	Marjoram ointment	153540	31991	60
Caelo	Marjoram ointment	160687	32516	40
Caelo	Marjoram ointment	162575	32872	40
Caelo	Marjoram ointment	162576	32873	40
Caelo	Marjoram ointment	181900	34259	40
Caelo	Marjoram ointment	22003319	36679	40
Fagron	Marjoram ointment	18L18-T07-062832	34418	40
Jenapharm	Neribas [®] fat ointment	YY011K0	32764	40
Jenapharm	Neribas [®] fat ointment	YY019KR	33290	40
Karo Pharma GmbH	Neribas [®] fat ointment	YY04F1L	35479	40
Caelo	Protegin [®] XN	161645	32340	40
Caelo	Protegin [®] XN	21003187003	36045	40
Chiesi	Asche Basis [®] fat ointment	53021A	32716	40
Chiesi	Asche Basis [®] fat ointment	53021A	32925	40

- 29 780 spectra from a total of 677 batches from further 205 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 1200 spectra from 392 *Apo-Ident* customers from 290 batches from the substance/substance group *Fat ointments*.
- Among them are spectra of independent samples from 275 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Protegin [®] XN	22000510002	1
	Protegin [®] XN	22000510005	1
	Protegin [®] XN	22000510011	2
	Protegin [®] XN	23001097004	4
	Protegin [®] XN	23001097005	3
	Protegin [®] XN	23001097007	3
	Protegin [®] XN	23002995001	3
	Protegin [®] XN	23002995003	3
	Protegin [®] XN	23002995007	6

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Supplier	Substance	Batch	Spectra
	Protegin [®] XN	23002995008	2
	Neribas [®] fat ointment	23IS8A	3
	Protegin [®] XN	24001198002	4
	Protegin [®] XN	24001198004	1
	Asche Basis [®] fat ointment	24009A	1
	Neribas [®] fat ointment	24B24A	3
	Protegin [®] XN	2711E-03598	1
	Asche Basis [®] fat ointment	33011A	1
	Asche Basis [®] fat ointment	41013A	3
	Neribas [®] fat ointment	6696045	1
Lamotte/ Noweda	Marjoram ointment	5322500	1
/ AHD	Neribas [®] fat ointment	YY016LP	2
22000510003	Protegin [®] XN	22000510003	2
Alliance / Fargon	Marjoram ointment	19G04-T03-069133	2
Alliance Healthcare	Marjoram ointment	21000565001	1
Alliance Healthcare	Protegin [®] XN	21003187003	1
Alliance Healthcare	Neribas [®] fat ointment	YY0431T	1
Bayer	Neribas [®] fat ointment	YY02L7L	1
BAYER/Phönix WE:26.0...	Neribas [®] fat ointment	YY011K0	1
Caelo	Protegin [®] XN	20001749003	1
	Marjoram ointment	10111402	1
Caelo	Protegin [®] XN	11022403	1
Caelo	Marjoram ointment	11061201	1
Caelo	Protegin [®] XN	11196702	2
Caelo	Protegin [®] XN	11196801	1
Caelo	Protegin [®] XN	11196802	1
Caelo	Protegin [®] XN	11196805	1
Caelo	Marjoram ointment	11274603	2
Caelo	Marjoram ointment	11327501	2
Caelo	Marjoram ointment	12018001	4
Caelo	Marjoram ointment	12018101	3
Caelo	Marjoram ointment	12081002	5
Caelo	Marjoram ointment	12123001	7
Caelo	Marjoram ointment	12123101	2
Caelo	Marjoram ointment	1213001	1
Caelo	Protegin [®] XN	12229201	5
Caelo	Protegin [®] XN	12229209	1
Caelo	Protegin [®] XN	12229210	1
Caelo	Protegin [®] XN	12229211	5
Caelo	Marjoram ointment	1225402	1
Caelo	Marjoram ointment	12295402	6
Caelo	Marjoram ointment	13028301	2
Caelo	Marjoram ointment	13028302	3
Caelo	Marjoram ointment	13028401	9
Caelo	Marjoram ointment	13051304	1
Caelo	Protegin [®] XN	13081901	4
Caelo	Protegin [®] XN	13081902	3
Caelo	Protegin [®] XN	13081903	1
Caelo	Protegin [®] XN	13081904	2
Caelo	Protegin [®] XN	13081905	11
Caelo	Protegin [®] XN	13081906	6
Caelo	Protegin [®] XN	13081907	3
Caelo	Protegin [®] XN	13081908	1
Caelo	Protegin [®] XN	13091906	1
Caelo	Marjoram ointment	13095401	5
Caelo	Marjoram ointment	13307102	6
Caelo	Protegin [®] XN	13344401	6

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Supplier	Substance	Batch	Spectra
Caelo	Protegin [®] XN	13344402	11
Caelo	Marjoram ointment	13382901	1
Caelo	Marjoram ointment	13382902	1
Caelo	Marjoram ointment	13382903	2
Caelo	Marjoram ointment	13383001	1
Caelo	Marjoram ointment	13e10-t04-003550	1
Caelo	Marjoram ointment	140020101	1
Caelo	Marjoram ointment	14002101	16
Caelo	Marjoram ointment	14089901	8
Caelo	Marjoram ointment	14090002	10
Caelo	Protegin [®] XN	14220201	1
Caelo	Protegin [®] XN	14220202	5
Caelo	Protegin [®] XN	14220203	3
Caelo	Protegin [®] XN	14220204	3
Caelo	Protegin [®] XN	14220205	6
Caelo	Protegin [®] XN	14220206	2
Caelo	Protegin [®] XN	14220208	4
Caelo	Protegin [®] XN	14220209	4
Caelo	Marjoram ointment	14332101	10
Caelo	Marjoram ointment	14332202	1
Caelo	Protegin [®] XN	14341301	3
Caelo	Protegin [®] XN	14341302	1
Caelo	Marjoram ointment	15038303	2
Caelo	Marjoram ointment	15038401	2
Caelo	Marjoram ointment	15038501	4
Caelo	Marjoram ointment	15101205	1
Caelo	Marjoram ointment	1513E-02536	1
Caelo	Protegin [®] XN	15252702	2
Caelo	Protegin [®] XN	15252703	5
Caelo	Marjoram ointment	15353303	2
Caelo	Marjoram ointment	15354001	5
Caelo	Marjoram ointment	15392402	2
Caelo	Protegin [®] XN	16026701	6
Caelo	Protegin [®] XN	16026702	6
Caelo	Protegin [®] XN	16026703	3
Caelo	Protegin [®] XN	16026704	5
Caelo	Protegin [®] XN	16026706	1
Caelo	Protegin [®] XN	16026707	6
Caelo	Protegin [®] XN	16026709	3
Caelo	Marjoram ointment	16068602	6
Caelo	Marjoram ointment	16068701	6
Caelo	Marjoram ointment	16068801	3
Caelo	Marjoram ointment	16068901	8
Caelo	Protegin [®] XN	16164501	1
Caelo	Protegin [®] XN	16164502	2
Caelo	Protegin [®] XN	16164503	2
Caelo	Protegin [®] XN	16164504	1
Caelo	Protegin [®] XN	16164505	6
Caelo	Protegin [®] XN	16164506	2
Caelo	Protegin [®] XN	16164507	1
Caelo	Marjoram ointment	16257502	3
Caelo	Marjoram ointment	16257602	5
Caelo	Marjoram ointment	16K07-T20-038496	1
Caelo	Marjoram ointment	17070901	11
Caelo	Marjoram ointment	17071001	6
Caelo	Marjoram ointment	17071101	14
Caelo	Protegin [®] XN	17256702	1
Caelo	Protegin [®] XN	17258702	1

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Supplier	Substance	Batch	Spectra
Caelo	Protegin [®] XN	17258703	3
Caelo	Protegin [®] XN	17258705	1
Caelo	Protegin [®] XN	17258707	3
Caelo	Protegin [®] XN	17258708	2
Caelo	Marjoram ointment	17302401	7
Caelo	Marjoram ointment	17302402	2
Caelo	Cottonwood ointment	18019902	1
Caelo	Marjoram ointment	18050901	7
Caelo	Marjoram ointment	18050902	5
Caelo	Protegin [®] XN	1805901	1
Caelo	Protegin [®] XN	1805907	1
Caelo	Protegin [®] XN	18059501	13
Caelo	Protegin [®] XN	18059502	11
Caelo	Protegin [®] XN	18059503	2
Caelo	Protegin [®] XN	18059505	1
Caelo	Protegin [®] XN	18059507	7
Caelo	Protegin [®] XN	18059509	1
Caelo	Protegin [®] XN	18059511	2
Caelo	Protegin [®] XN	18059512	4
Caelo	Marjoram ointment	18190001	15
Caelo	Marjoram ointment	18190101	5
Caelo	Marjoram ointment	18190102	5
Caelo	Marjoram ointment	18251602	2
Caelo	Marjoram ointment	18251603	1
Caelo	Marjoram ointment	18D11-T01-054700	1
Caelo	Marjoram ointment	19033001	19
Caelo	Marjoram ointment	1903301	1
Caelo	Marjoram ointment	19033101	4
Caelo	Marjoram ointment	19033102	18
Caelo	Marjoram ointment	19033120	1
Caelo	Protegin [®] XN	191090001	1
Caelo	Protegin [®] XN	19109001	5
Caelo	Protegin [®] XN	19109002	21
Caelo	Protegin [®] XN	19109003	2
Caelo	Protegin [®] XN	1910920002	1
Caelo	Protegin [®] XN	191092002	7
Caelo	Protegin [®] XN	191092002/4820	1
Caelo	Protegin [®] XN	19110201	9
Caelo	Protegin [®] XN	19110202	21
Caelo	Marjoram ointment	19115102	2
Caelo	Marjoram ointment	19115103	6
Caelo	Marjoram ointment	200000282001	1
Caelo	Protegin [®] XN	200001749005	1
Caelo	Marjoram ointment	20000281001	17
Caelo	Marjoram ointment	20000282001	16
Caelo	Marjoram ointment	20000283001	1
Caelo	Marjoram ointment	20000283002	10
Caelo	Marjoram ointment	20000283003	5
Caelo	Marjoram ointment	200002853002	1
Caelo	Marjoram ointment	2000082001	1
Caelo	Protegin [®] XN	2000149012	1
Caelo	Protegin [®] XN	20001749001	5
Caelo	Protegin [®] XN	20001749003	8
Caelo	Protegin [®] XN	20001749004	2
Caelo	Protegin [®] XN	20001749005	2
Caelo	Protegin [®] XN	20001749007	8
Caelo	Protegin [®] XN	20001749010	7
Caelo	Protegin [®] XN	20001749012	2

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Supplier	Substance	Batch	Spectra
Caelo	Protegin [®] XN	20001749013	2
Caelo	Cottonwood ointment	20002385002	1
Caelo	Marjoram ointment	20003044001	10
Caelo	Marjoram ointment	2000304401	1
Caelo	Marjoram ointment	20003045001	14
Caelo	Marjoram ointment	20003045002	1
Caelo	Protegin [®] XN	20011402	1
Caelo	Protegin [®] XN	2001749003	1
Caelo	Marjoram ointment	2003045001	1
Caelo	Marjoram ointment	2011405	1
Caelo	Marjoram ointment	2021506	1
Caelo	Marjoram ointment	20290312-1	1
Caelo	Marjoram ointment	21000565001	14
Caelo	Protegin [®] XN	21003187001	7
Caelo	Protegin [®] XN	21003187003	6
Caelo	Protegin [®] XN	21003187005	1
Caelo	Protegin [®] XN	21003187006	3
Caelo	Marjoram ointment	210809(20000282001)	1
Caelo	Marjoram ointment	22000091001	6
Caelo	Marjoram ointment	22000091003	2
Caelo	Protegin [®] XN	22000510002	1
Caelo	Protegin [®] XN	22000510004	4
Caelo	Protegin [®] XN	22000510005	1
Caelo	Protegin [®] XN	22000510007	2
Caelo	Marjoram ointment	22003319001	7
Caelo	Marjoram ointment	22003319002	3
Caelo	Marjoram ointment	220728(20000283002)	1
Caelo	Protegin [®] XN	25061301	1
Caelo	Protegin [®] XN	26031509	1
Caelo	Marjoram ointment	27031505	1
Caelo	Protegin [®] XN	3091208	1
Caelo	Marjoram ointment	312115354001	1
Caelo	Marjoram ointment	312200030451	1
Caelo	Marjoram ointment	5322500	1
Caelo	Protegin [®] XN	6012014A	1
Caelo	Marjoram ointment	64(17071001)	1
Caelo	Marjoram ointment	65(17070901)	1
Caelo	Marjoram ointment	66(18050902)	1
Caelo	Marjoram ointment	66(18190001)	1
Caelo	Marjoram ointment	7121203	1
Caelo	Asche Basis [®] fat ointment	73025A	3
Caelo	Marjoram ointment	8031304	1
Caelo	Protegin [®] XN	8031305	1
Caelo	Neribas [®] fat ointment	yy00k7C	1
Caeolo	Marjoram ointment	14090002	1
Caeolo	Marjoram ointment	1539402	1
Caesar & Lorenz Sanacorp	Marjoram ointment	19033102	1
Caesar & Loretz GmbH...	Protegin [®] XN	19110202	2
Caesar & Loretz GmbH...	Protegin [®] XN	22000510002	1
Caesar & Loretz GmbH...	Protegin [®] XN	19110201	1
Caesar & Loretz GmbH	Protegin [®] XN	16164506	1
Caesar & Loretz GmbH	Protegin [®] XN	18059501	1
Caesar & Loretz GmbH	Protegin [®] XN	18059507	1
Caesar & Loretz GmbH	Protegin [®] XN	18059511	1
Caesar & Loretz GmbH	Protegin [®] XN	18059512	3
Caesar & Loretz GmbH	Marjoram ointment	19033001	1
Caesar & Loretz GmbH	Marjoram ointment	19033102	1
Caesar & Loretz GmbH	Protegin [®] XN	191090001	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Protegin [®] XN	19109001	1
Caesar & Loretz GmbH	Protegin [®] XN	19109002	16
Caesar & Loretz GmbH	Protegin [®] XN	191092001	1
Caesar & Loretz GmbH	Protegin [®] XN	19110201	2
Caesar & Loretz GmbH	Protegin [®] XN	19110202	9
Caesar & Loretz GmbH	Marjoram ointment	19115102	1
Caesar & Loretz GmbH	Marjoram ointment	20000281001	5
Caesar & Loretz GmbH	Protegin [®] XN	20001749001	2
Caesar & Loretz GmbH	Protegin [®] XN	20001749003	6
Caesar & Loretz GmbH	Protegin [®] XN	20001749005	3
Caesar & Loretz GmbH	Protegin [®] XN	20001749007	5
Caesar & Loretz GmbH	Protegin [®] XN	20001749010	1
Caesar & Loretz GmbH	Protegin [®] XN	20001749012	1
Caesar & Loretz GmbH	Marjoram ointment	20003044001	2
Caesar & Loretz GmbH	Marjoram ointment	20003045001	2
Caesar & Loretz GmbH	Marjoram ointment	21000565001	1
Caesar & Loretz GmbH	Protegin [®] XN	21003187001	1
Caesar & Loretz GmbH	Protegin [®] XN	21003187003	4
Caesar & Loretz GmbH	Protegin [®] XN	21003187006	1
Caesar & Loretz GmbH	Protegin [®] XN	22000510002	1
Caesar & Loretz GmbH	Protegin [®] XN	22000510004	2
Caesar & Loretz GmbH	Protegin [®] XN	22000510009	1
Caesar & Loretz GmbH	Marjoram ointment	22003319002	1
Caesar & Loretz GmbH...	Protegin [®] XN	21003187006	1
Caesar & Loretz GmbH...	Protegin [®] XN	22000510002	1
Caesar & Loretz GmbH...	Protegin [®] XN	18059507	1
Caesar & Loretz GmbH...	Protegin [®] XN	21003187001	2
Caesar & Loretz GmbH/Gehe	Marjoram ointment	18190001	2
Caesar & Loretz GmbH/Gehe	Marjoram ointment	20000283003	1
Caesar & Loretz GmbH/Gehe	Marjoram ointment	21000565001	1
Caesar & Loretz GmbH/Gehe	Protegin [®] XN	22000510004	1
Caesar & Loretz GmbH...	Protegin [®] XN	19110202	1
Caesar & Loretz GmbH...	Marjoram ointment	20000281001	1
Caesar & Loretz GmbH...	Marjoram ointment	20000282001	1
Caesar & Loretz GmbH...	Marjoram ointment	20003044001	1
Caesar & Loretz GmbH/Kehr	Protegin [®] XN	22000510002	2
Caesar & Loretz GmbH...	Protegin [®] XN	19109001	1
Caesar & Loretz GmbH...	Protegin [®] XN	20001749010	1
Caesar & Loretz GmbH...	Protegin [®] XN	20001749013	1
Caesar & Loretz GmbH...	Protegin [®] XN	19109003	1
Caesar & Loretz GmbH...	Protegin [®] XN	20001749004	1
Caesar & Loretz GmbH...	Protegin [®] XN	20001749009	2
Caesar & Loretz GmbH...	Protegin [®] XN	21003187001	2
Caesar & Loretz GmbH...	Protegin [®] XN	21003187003	1
Caesar & Loretz GmbH...	Marjoram ointment	19033102	1
Caesar & Loretz GmbH...	Marjoram ointment	19115103	1
Caesar & Loretz GmbH...	Marjoram ointment	20003045001	1
Caesar & Loretz	Cottonwood ointment	19012902	1
Caesar & Loretz	Protegin [®] XN	19109001	1
Caesar & Loretz	Protegin [®] XN	19110201	1
Caleo/ Noweda	Marjoram ointment	17302401	1
Caleo/ Noweda	Marjoram ointment	17302402	2
Cealo	Marjoram ointment	13028401	2
Cealo	Marjoram ointment	20003045001	1
Cealo/Jenne	Marjoram ointment	220323(20000283002)	1
Cealo/Noweda	Protegin [®] XN	18059505	1
Cealo/Noweda	Protegin [®] XN	20001749012	1

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Supplier	Substance	Batch	Spectra
Chiese	Asche Basis [®] fat ointment	33016A	1
Chiese	Asche Basis [®] fat ointment	63023A	1
Chiesi GmbH	Asche Basis [®] fat ointment	14007A	1
Chiesi GmbH/Phönix	Asche Basis [®] fat ointment	93029A	2
Chiesi Sanacorp	Asche Basis [®] fat ointment	82027A	1
CHiesi	Asche Basis [®] fat ointment	41018A	3
Chiesi	Asche Basis [®] fat ointment	51020A	1
Chiesi	Asche Basis [®] fat ointment	63023A	1
Chiesi	Asche Basis [®] fat ointment	81026A	1
Chiesi	Asche Basis [®] fat ointment	82027A	1
Chiesi	Asche Basis [®] fat ointment	84028A	1
Chiesi/ Noweda	Asche Basis [®] fat ointment	82027A	1
Chiesi/ Sanacorp	Asche Basis [®] fat ointment	2001A	1
Chiesi/ Sanacorp	Asche Basis [®] fat ointment	84028A	1
Chiesi/ Sanacorp	Asche Basis [®] fat ointment	93029A	1
Chiesi/Gehe	Asche Basis [®] fat ointment	41017A	1
Chiesi/Gehe	Asche Basis [®] fat ointment	51020A	1
Chiesi/Jenne	Asche Basis [®] fat ointment	24010A	1
Chiesi/Noweda	Asche Basis [®] fat ointment	82027A	1
Chiesi/Phönix	Asche Basis [®] fat ointment	73025A	1
Deumavan/Phoenix	Deumavan [®] protection oint...	21710920	1
Elbdeich Apotheke oc...	Neribas [®] fat ointment	YY04f1L	1
Euro OTC	Protegin [®] XN		1
Fagron	Marjoram ointment	12081002	1
Fagron	Marjoram ointment	12d24-t01	1
Fagron	Marjoram ointment	12D24-T01	2
Fagron	Marjoram ointment	12D24-T02	1
Fagron	Marjoram ointment	13a16-0001	1
Fagron	Marjoram ointment	13A16-T02	1
Fagron	Marjoram ointment	13A16-T04-000208	1
Fagron	Marjoram ointment	13A16-To4-000208	1
Fagron	Marjoram ointment	13F27-T03-004962	3
Fagron	Marjoram ointment	13F27-To3-004962	2
Fagron	Marjoram ointment	14090002	1
Fagron	Marjoram ointment	14A07-T04-009079	3
Fagron	Marjoram ointment	14a07-T04009079	1
Fagron	Marjoram ointment	14A07-T05-009082	2
Fagron	Marjoram ointment	14A07-T06-009085	3
Fagron	Marjoram ointment	15K10-T10-027644	3
Fagron	Marjoram ointment	16E02-T02-032846	1
Fagron	Marjoram ointment	16K07-T20-038496	4
Fagron	Marjoram ointment	17B03-T02-041256	2
Fagron	Marjoram ointment	17E22-T09-044517	2
Fagron	Protegin [®] XN	18059501	1
Fagron	Protegin [®] XN	18059507	1
Fagron	Marjoram ointment	18D11-T01-054700	1
Fagron	Marjoram ointment	18Dn-T01-054700	1
Fagron	Marjoram ointment	18L18-T07-062832	6
Fagron	Marjoram ointment	19G04-T03	1
Fagron	Marjoram ointment	19G04-T03-069133	4
Fagron	Marjoram ointment	T03-0691303	1
Fargon - Alliance He...	Marjoram ointment	18D11-T01-054700	1
Gehe	Protegin [®] XN	12229201	1
Gehe	Protegin [®] XN	12229211	1
Gehe	Marjoram ointment	13307102	1
Gehe	Marjoram ointment	14090002	1
Gehe	Marjoram ointment	15038501	1
Gehe	Marjoram ointment	15354001	1

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Supplier	Substance	Batch	Spectra
Gehe	Protegin [®] XN	16026701	2
Gehe	Marjoram ointment	16257602	2
Gehe	Marjoram ointment	17071001	1
GEHE	Protegin [®] XN	18059507	1
Gehe	Marjoram ointment	18190102	5
Gehe	Marjoram ointment	19033001	1
Gehe	Marjoram ointment	20000282001	1
Gehe	Marjoram ointment	21000565001	1
Gehe	Protegin [®] XN	23001097005	1
Gehe/La Motte	Marjoram ointment	5563400	1
GP Grenzach Produkti...	Neribas [®] fat ointment	YY00K7C	1
Hedinger/Phönix	Protegin [®] XN	18059501	1
Hedinger/Sanacorp	Neribas [®] fat ointment	YY01TF2	2
Henry Lamotte GmbH/H...	Marjoram ointment	5067400	1
Henry Lamotte Oils G...	Marjoram ointment	5067400	1
Henry Lamotte Oils GmbH	Marjoram ointment	5322500	1
Henry Lamotte Oils GmbH	Marjoram ointment	5563400	1
Henry Lamotte Oils G...	Marjoram ointment	5322500	1
Henry Lamotte Oils	Marjoram ointment	5067400	1
Henry Lamotte	Marjoram ointment	5563400	1
Ichthyl-Gesellschaft	Protegin [®] XN	17258703	1
Jenapharm / Fiebig	Neribas [®] fat ointment	YY01TF2	1
Jenapharm /Gehe	Neribas [®] fat ointment	YY0282F	1
Jenapharm	Neribas [®] fat ointment	YY016LP	1
Jenapharm	Neribas [®] fat ointment	YY01TF2	1
Jenapharm	Neribas [®] fat ointment	YY0282F	1
Jenapharm	Neribas [®] fat ointment	YY02L7L	1
Jenapharm	Neribas [®] fat ointment	YY0431T	1
Jenapharm/	Neribas [®] fat ointment	YY011K0	1
Jenapharm/AHCA	Neribas [®] fat ointment	YY0282F	2
Jenapharm/AHCA	Neribas [®] fat ointment	YY02L7L	2
Jenapharm/Ahd	Neribas [®] fat ointment	YY011Ko	1
Jenapharm/Anzag	Neribas [®] fat ointment	YY0282F	1
Jenapharm/Gehe	Neribas [®] fat ointment	YY01PFP	1
Jenapharm/Krieger	Neribas [®] fat ointment	YY0282F	3
Jenapharm/Krieger	Neribas [®] fat ointment	YY02L7L	3
Jenapharm/Noweda	Neribas [®] fat ointment	YY01TF2	1
Jenapharm/Phönix	Neribas [®] fat ointment	YY0282F	1
Jenapharm/Phönix	Neribas [®] fat ointment	YY00K7C	1
Jenne	Marjoram ointment	13028302	2
Jenne	Cottonwood ointment	17057404	1
Karo Pharma / Phoenix	Neribas [®] fat ointment	YY04F1L	1
Karo Pharma	Neribas [®] fat ointment	22AB1/75	1
Karo Pharma	Neribas [®] fat ointment	YY04F1L	2
Karo Pharma	Neribas [®] fat ointment	YY04P2K	1
Karo Pharma	Neribas [®] fat ointment	YY054E8	1
Karo Pharma/ Gehe	Neribas [®] fat ointment	YY04F1L	6
Karo Pharma/ Gehe	Neribas [®] fat ointment	YY04P2K	4
Karo Pharma/ Gehe	Neribas [®] fat ointment	YY04P2K	1
Karo Pharma/ Sanacorp	Neribas [®] fat ointment	YY04P2K	1
Karo Pharma/ sanacorp	Neribas [®] fat ointment	YY054E8	1
KARO PHARMA/Gehe	Neribas [®] fat ointment	YY04P2K	1
Karo Pharma/Gehe	Neribas [®] fat ointment	YY054E8	1
Karo Pharma/Phoenix	Neribas [®] fat ointment	YY04P2K	1
Karo Pharma/Phönix	Neribas [®] fat ointment	YY054E8	1
Karo	Neribas [®] fat ointment	YY054E8	1
Kaymogyn GmbH / Phoenix	Deumavan [®] protection oint...	LOT25620721	1

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Supplier	Substance	Batch	Spectra
Kaymogyn GmbH	Deumavan [®] protection oint...	21710920	1
Kehr	Marjoram ointment	17071101	1
Kehr	Protegin [®] XN	1805607	1
Klenk	Protegin [®] XN	18059502	1
krieger	Protegin [®] XN	19110202	1
Lamotte / Gehe	Marjoram ointment	5322500	1
Lamotte/Alliance	Marjoram ointment	5563400	3
Lamotte/Sanacorp	Marjoram ointment	5563400	1
Leo Pharma / Phönix	Neribas [®] fat ointment	YY0431T	1
Leo Pharma A/S / Phönix	Neribas [®] fat ointment	YY0431T	1
LEO Pharma A/S	Neribas [®] fat ointment	YY04311	1
leo Pharma	Neribas [®] fat ointment	yy0431T	1
Leo Pharma	Neribas [®] fat ointment	YY0431T	1
Leo Pharma/ Sanacorp	Neribas [®] fat ointment	YY0431T	1
Leo Pharma/ Sanacorp	Neribas [®] fat ointment	YY04F1L	3
LEO Pharma/Alliance	Neribas [®] fat ointment	YY04F1L	1
LEO Pharma/Gehe	Neribas [®] fat ointment	YY0431T	1
Leo/ Gehe	Neribas [®] fat ointment	YY0431T	2
LeoPharma/Krieger	Neribas [®] fat ointment	YY04F1L	1
LeoPharma/Phönix	Neribas [®] fat ointment	YY0431T	1
Max Jenne	Protegin [®] XN	23002995008	1
Noweda	Protegin [®] XN	21003187002	1
Noweda	Protegin [®] XN	22000510002	1
Noweda	Marjoram ointment	2203319001	1
Noweda	Marjoram ointment	5322500	1
Noweda	Neribas [®] fat ointment	YY0282F	4
Noweda	Neribas [®] fat ointment	YY02L7L	1
Noweda	Neribas [®] fat ointment	YY02L7L	1
Phoenix WE 24.04.17 ...	Neribas [®] fat ointment	YY019KR	1
Phoenix	Marjoram ointment	13028401	1
Phoenix	Protegin [®] XN	19110202	1
Phoenix	Protegin [®] XN	20001749010	1
Phoenix	Protegin [®] XN	22000510007	2
Phoenix	Neribas [®] fat ointment	YY00K7C	1
phoenix/Karo Pharma	Neribas [®] fat ointment	YY04F1L	1
Phönix 10.12.12	Marjoram ointment	12D24-T02	1
Phönix 12.03.2013	Protegin [®] XN	12229205	1
Phönix, 07.11.13	Protegin [®] XN	12229210	1
Phönix	Protegin [®] XN	11196706	1
Phönix	Marjoram ointment	12018001	1
Phönix	Protegin [®] XN	13081901	3
Phönix	Protegin [®] XN	16026707	1
Phönix	Marjoram ointment	16068901	1
Phönix	Marjoram ointment	17071001	1
Phönix	Marjoram ointment	17302401	1
PHÖNIX	Protegin [®] XN	18059501	1
Phönix	Marjoram ointment	18190001	2
PHÖNIX	Marjoram ointment	19033101	1
Phönix	Protegin [®] XN	20001749004	1
phönix	Protegin [®] XN	23002995006	1
Phönix	Protegin [®] XN	23002995008	1
PhönixWE:18.01.2017 ...	Neribas [®] fat ointment	YY016LP	1
Römerapo.	Neribas [®] fat ointment	YY01TF2	1
Sanacorp 05.10.21 EK...	Marjoram ointment	211019UM	1
Sanacorp, 21.03.17, 5,73EUR	Marjoram ointment	16068602	1
Sanacorp	Marjoram ointment	12081002	1
Sanacorp	Marjoram ointment	12295402	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Marjoram ointment	13095401	1
Sanacorp	Marjoram ointment	15038401	1
Sanacorp	Marjoram ointment	16257502	2
Sanacorp	Protegin® XN	22000510011	1
Sanacorp	Protegin® XN	23001097005	1
Sanacorp	Marjoram ointment	5563400	1
Spangropharm	Marjoram ointment	4961000	1
VDL	Marjoram ointment	14090002	1

- 19 578 spectra from 1526 *Apo-Ident* customers from a total of 6064 batches from a further 161 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	1120	0	26 814
Type B	0	1150	0	29 620
Type C	0	1195	5	19 578

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9613 %)	100.0000 % (> 99.4643 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 99.4783 %)
Type C	100.0000 % (> 99.0582 %)	99.5833 % (> 99.3333 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30881	30881	0.00	32.59
30926	30926	0.00	34.52
31013	31013	0.00	31.39
31112	31112	0.00	28.26
31443	31443	0.00	33.40
31475	31475	0.00	24.85
31489	31489	0.00	37.92
31858	31858	0.00	37.88
31872	31872	0.00	39.39
32473	32473	0.00	30.25
33130	33130	0.00	30.38
33131	33131	0.00	31.92
33634	33634	0.00	32.23
33921	33921	0.00	29.54
33986	33986	0.00	38.39
34783	34783	0.00	35.34
34963	34963	0.00	31.97
34966	34966	0.00	30.16
34967	34967	0.00	30.37
35069	35069	0.00	20.26
35071	35071	0.00	20.16
35346	35346	0.00	30.01
35471	35471	0.00	36.23
36144	36144	0.00	30.84
36671	36671	0.00	31.53
36744	36744	0.00	18.81
38641	38641	0.00	33.61

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Fennel oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31140-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Fennel oil; Oleum foeniculum vulgare var. dulce

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Fennel oil	4	2	2

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fennel oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Anise oil, organic	16.15	—
Cumin oil	59.10	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Fennel oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Fennel oil	L16813D-111973BAG90451	31140	40	not required
Taoasis	Fennel oil	L35513DN-119762	31693	60	not required
Taoasis	Fennel oil	1806-125039	32795	40	not required
Taoasis	Fennel oil	L14218DN-17142	37662	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Fennel oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 754 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are

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

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Fennel oil	1806-127213	32952	40
Taoasis	Fennel oil	1861-129086	33991	40

- 30 850 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Fennel oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis	Fennel oil	2307-5296	1
Taoasis	Fennel oil	2307-7139	1

- 20 776 spectra from 1559 *Apo-Ident* customers from a total of 6350 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	180	0	27 754
Type B	0	73	7	30 850
Type C	0	2	0	20 776

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9567 %)	91.2500 % (> 87.5000 %)
Type C	100.0000 % (> 99.0834 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31140	31140	0.00	93.06
31693	31693	0.00	91.60
32795	32795	0.00	20.97
37662	37662	0.00	89.62

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Ginger oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30451-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Ginger oil; Oleum zingiber officinalis

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Ginger oil	4	3	6

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ginger oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citus oil	18.01	—
Frankincense oil	18.09	—
Hyssop oil	19.71	—
Vetiver bourbon oil	19.75	—
Myrtle oil	22.38	—
Marjoram oil	23.75	—
Angelica root oil	24.94	—
Cedar wood oil	25.01	—
Lemon grass oil	25.26	—
Immortelle oil	26.28	—
Cypress oil	32.51	—
Pine silvestris oil	33.26	—
Cumin oil	33.52	—
Dwarf pine oil	38.96	—
Yarrow oil	39.16	—
Spearmint oil	39.80	—
Carrot seed oil	41.20	—
Spruce needle oil	42.11	—
Camphor oil	42.68	—
Matricaria oil, morrocan	45.18	—
Manuka oil	46.29	—
Swiss pine oil	47.59	—
Silver fir oil	49.94	—
Rosemary oil	51.92	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Ginger oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Ginger oil	00552A27	34407	40	not required
Taoasis	Ginger oil	130114-110686BAG90451	30958	40	not required
Taoasis	Ginger oil	40592A-112718BAG90451	31142	40	not required
Taoasis	Ginger oil	1431020-124656	32270	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Ginger oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 774 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 160 spectra of 4 reference samples from the substance/substance group *Ginger oil*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Bombastus	Ginger oil	300690	32569	40
Bombastus	Ginger oil	22000860	36888	40
Taoasis	Ginger oil	19008	38598	40
Bombastus	Ginger oil	300690	33014	40

- 30 770 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

provided by the customer regarding manufacturer and batch number.

- 8 spectra from 3 *Apo-Ident* customers from 6 batches from the substance/substance group *Ginger oil*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ginger oil	5684-13176	1
Primavera	Ginger oil	371G27	1
Primavera	Ginger oil	99D28	1
Taoasis	Ginger oil	6454-92725	1
Taoasis	Ginger oil	6971-14345	3
Taoasis	Ginger oil	697114345	1

- 20 770 spectra from 1559 *Apo-Ident* customers from a total of 6346 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	160	0	27 774
Type B	0	160	0	30 770
Type C	0	8	0	20 770

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9618 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.0645 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30958	30958	0.00	19.71
31142	31142	0.00	23.22
32270	32270	0.00	29.04
34407	34407	0.00	28.88

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Grapefruit oil organic / Orange oil / Blood orange oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30960-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Grapefruit oil organic / Orange oil / Blood orange oil; Blood orange oil; Grapefruit oil, organic; Oleum citrus paradisi; Oleum citrus sinensis; Orange oil

Special notes

When selecting the *Grapefruit oil organic / Orange oil / Blood orange oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Grapefruit oil organic / Orange oil / Blood orange oil	8	16	55

Second-stage model

For differentiation of the substance/substance group *Grapefruit oil organic / Orange oil / Blood orange oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Grapefruit oil organic / Orange oil / Blood orange oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citric oil	17.45	—
Mandarin oil, green	46.73	—
Lime oil	61.09	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Grapefruit oil organic / Orange oil / Blood orange oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Blood orange oil	00413G25	33761	40	not required
Taoasis	Blood orange oil	494J09	33759	40	not required
Apotheker ...	Grapefruit oil, organic	7.99615.16.02	31853	60	not required
Taoasis	Grapefruit oil, organic	31564-119383	31634	120	not required
Taoasis	Grapefruit oil, organic	38755-122181	31781	60	not required
Primavera	Orange oil	00112K25	33805	40	not required
Taoasis	Orange oil	121109-110685BAG90451	30960	40	not required
Taoasis	Orange oil	33732-12088	31679	60	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 460 spectra of 8 reference samples from the substance/substance group *Grapefruit oil organic / Orange oil / Blood orange oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 8 different batches.
- 27 474 spectra from a total of 592 batches from further 141 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 631 spectra of 16 reference samples from the substance/substance group *Grapefruit oil organic / Orange oil / Blood orange oil*.
- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Blood orange oil	00318C26	34175	40
Primavera	Blood orange oil	00111H26	34296	31
Primavera	Blood orange oil	00013A27	34376	40
Taoasis	Blood orange oil	17021-IT-R04	37652	40
Apotheker Bauer & Cie	Grapefruit oil, organic	7.68413.17.012018-03	33019	40
Primavera	Grapefruit oil, organic	00553M26	34385	40
Taoasis	Grapefruit oil, organic	44040A-124468	32979	40
Taoasis	Grapefruit oil, organic	12761A-16417	37648	40
Primavera	Orange oil	00149A29	33956	40
Primavera	Orange oil	00058G26	34180	40
Primavera	Orange oil	00729L26	34392	40
Primavera	Orange oil	00772E31	37786	40
Taoasis	Orange oil	43829C-124974	32790	40
Taoasis	Orange oil	44583A-126780	32902	40
Taoasis	Orange oil	011855A-1538	34105	40
Taoasis	Orange oil	050509A-16471	37689	40

- 30 299 spectra from a total of 693 batches from further 208 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 58 spectra from 17 *Apo-Ident* customers from 56 batches from the substance/substance group *Grapefruit oil organic / Orange oil / Blood orange oil*.
- Among them are spectra of independent samples from 55 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Orange oil	21005346	1
	Orange oil	22005052	1
	Orange oil	23004146	1
	Orange oil	23004392	2
	Orange oil	24003140	1
	Orange oil	24004443	1
BerglandSanacorp	Orange oil	K602772	1
Bombastus	Orange oil	20005182	1
Bombastus	Orange oil	298756	1
Bombastus	Orange oil	302428	1
Caelo	Orange oil		1
Caelo	Orange oil	19113809	1
Caelo	Grapefruit oil, organic	21003280003	1
noweda	Orange oil	P202107	1
Primavera, Gehe	Orange oil	131A27	1
Primavera, Gehe	Orange oil	171F28	1
Primavera, Gehe	Blood orange oil	576J27	1
Primavera, Gehe	Orange oil	741E29	1
Primavera, Gehe	Orange oil	890G25	1
Primavera	Blood orange oil	378H29	1
Primavera	Blood orange oil	431L28	1
Primavera	Orange oil	449H31	1
Primavera	Orange oil	471M30	1
Taoasis	Orange oil	11855A-3824	1
Taoasis	Orange oil	122650-123643	1
Taoasis	Orange oil	140129-116983	1
Taoasis	Orange oil	140129-118141	1
Taoasis	Orange oil	140129-118420	1
Taoasis	Orange oil	140129-118790	1
Taoasis	Blood orange oil	1AR18M-3519	1
Taoasis	Grapefruit oil, organic	25011-9210	1
Taoasis	Grapefruit oil, organic	253030-10699	1
Taoasis	Grapefruit oil, organic	31564-120540	1
Taoasis	Grapefruit oil, organic	40038-123110	1
Taoasis	Orange oil	42861A-121691	1
Taoasis	Orange oil	42861A-122532	1
Taoasis	Orange oil	43829C-124155	1
Taoasis	Orange oil	43829C-125351	1
Taoasis	Grapefruit oil, organic	44040A-124467	1
Taoasis	Grapefruit oil, organic	44040A-124468	1
Taoasis	Grapefruit oil, organic	44040A-127409	1
Taoasis	Orange oil	44583A-128241	1
Taoasis	Orange oil	45441A-1035	1
Taoasis	Orange oil	45451A-1178	1
Taoasis	Orange oil	45451A-128935	1
Taoasis	Grapefruit oil, organic	46701-128853	1
Taoasis	Grapefruit oil, organic	47037-1144	2
Taoasis	Grapefruit oil, organic	47037-1602	1
Taoasis	Grapefruit oil, organic	47037-958	1
Taoasis	Orange oil	47450A-7457	1
Taoasis	Grapefruit oil, organic	48566-1955	1
Taoasis	Orange oil	6193	1
Taoasis	Grapefruit oil, organic	AR18-12022-6352	1
Taoasis/Gehe	Orange oil	497J09	1

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Supplier	Substance	Batch	Spectra
Taoasis/Taoasis	Grapefruit oil, organic	40238-123217	1
Taoasis/Taoasis	Orange oil	44583A-127488	1

- 20 720 spectra from 1558 *Apo-Ident* customers from a total of 6297 batches from a further 164 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	460	0	27 474
Type B	0	631	0	30 299
Type C	0	57	1	20 720

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9614 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9564 %)	100.0000 % (> 99.0491 %)
Type C	100.0000 % (> 99.0591 %)	98.2759 % (> 93.1034 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30960	30960	0.00	45.95
31634	31634	0.00	44.09
31679	31679	0.00	48.02

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31781	31781	0.00	48.65
31853	31853	0.00	38.90
33759	33759	0.00	46.26
33761	33761	0.00	45.65
33805	33805	0.00	46.77

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Immortelle oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30450-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Immortelle oil; Oleum helichrysum italicum

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Immortelle oil	5	2	6

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Immortelle oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Melissa oil	15.27	—
Ginger oil	16.05	—
Vetiver bourbon oil	18.24	—
Lemon grass oil	19.07	—
Cypress oil	24.58	—
Myrtle oil	24.77	—
Citus oil	28.43	—
Cedar wood oil	30.28	—
Chamomile (essential oil)	34.07	—
Manuka oil	35.21	—
Marjoram oil	35.69	—
Spearmint oil	36.08	—
Swiss pine oil	40.22	—
Dwarf pine oil	42.03	—
Hyssop oil	46.98	—
Patchouli oil	47.49	—
Cumin oil	51.21	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Immortelle oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Immortelle oil	00324A27	34383	40	not required
Taoasis	Immortelle oil	L24113D-113148BAG90451	31138	40	not required
Taoasis	Immortelle oil	L24415DN-122092BAG90451	32069	60	not required
Taoasis	Immortelle oil	114717DNJ-137	33727	40	not required
Taoasis	Immortelle oil	S20210929-17125	37798	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 5 reference samples from the substance/substance group *Immortelle oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 714 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Immortelle oil	L17716DN-126770	32975	40
Taoasis	Immortelle oil	L17716DN-124955	33021	40

- 30 850 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 7 spectra from 4 *Apo-Ident* customers from 6 batches from the substance/substance group *Immortelle oil*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis	Immortelle oil	7750IT-L08	1
Taoasis	Immortelle oil	L03111DN	1
Taoasis	Immortelle oil	L14520DN	1
Taoasis	Immortelle oil	L14717DNJ-132	1
Taoasis	Immortelle oil	L14717DNJ-3017	1
Taoasis	Immortelle oil	L38914DN-118878	2

- 20 771 spectra from 1559 *Apo-Ident* customers from a total of 6346 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	220	0	27 714
Type B	0	80	0	30 850
Type C	0	7	0	20 771

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0654 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31138	31138	0.00	25.32
32069	32069	0.00	21.32
33727	33727	0.00	27.33
34383	34383	0.00	24.60
37798	37798	0.00	29.88

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Juniper berry oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31559-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Juniper berry oil

Special notes

When selecting the *Juniper berry oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Juniper berry oil	5	3	2

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Juniper berry oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Spruce needle oil	9.56	—
Frankincense oil	11.16	—
Dwarf pine oil	19.20	—
Silver fir oil	21.79	—
Spearmint oil	23.96	—
Swiss pine oil	24.04	—
Pine silvestris oil	24.08	—
Angelica root oil	26.36	—
Cypress oil	33.77	—
Ginger oil	38.04	—
Citrus oil	38.43	—
Marjoram oil	38.68	—
Yarrow oil	39.97	—
Cumin oil	42.77	—
Matricaria oil, morrocan	43.33	—
Camphor oil	46.80	—
Bergamot oil	46.83	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Juniper berry oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Juniper berry oil	4155-116757	31559	60	not required
Taoasis	Juniper berry oil	4155-120900	31687	60	not required
Taoasis	Juniper berry oil	02JB0B-126047	32809	40	not required
Taoasis	Juniper berry oil	9321-14903	37674	40	not required
Taoasis	Juniper berry oil	19832	38785	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Juniper berry oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 694 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Juniper berry oil	00497L26	34398	40
Taoasis	Juniper berry oil	02JB0B-127283	32932	40
Taoasis	Juniper berry oil	1713-128196	33651	40

- 30 810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Juniper berry oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Juniper berry oil	16160706	1
Taoasis	Juniper berry oil	155-118896	1

- 20 776 spectra from 1559 *Apo-Ident* customers from a total of 6350 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	240	0	27 694
Type B	0	112	8	30 810
Type C	0	2	0	20 776

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9566 %)	93.3333 % (> 90.8333 %)
Type C	100.0000 % (> 99.0834 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31559	31559	0.00	25.75
31687	31687	0.00	27.32
32809	32809	0.00	23.43
37674	37674	0.00	18.64
38785	38785	0.00	9.56

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Lemon grass oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30661-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Lemon grass oil; Cymbopogonis aetheroleum

Special notes

When selecting the *Lemon grass oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Lemon grass oil	7	4	31

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lemon grass oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Immortelle oil	22.93	—
Marjoram oil	28.05	—
Vetiver bourbon oil	28.26	—
Cypress oil	29.48	—
Melissa oil	30.30	—
Carrot seed oil	33.73	—
Patchouli oil	35.48	—
Tea tree oil	38.17	—
Myrtle oil	39.55	—
Ginger oil	39.86	—
Cedar wood oil	42.20	—
Citrus oil	47.55	—
Dwarf pine oil	51.19	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Lemon grass oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Bombastus	Lemon grass oil	263571	30661	40	not required
Bombastus	Lemon grass oil	278923	31185	40	not required
Bombastus	Lemon grass oil	278526	31187	40	not required
Bombastus	Lemon grass oil	20003469	36040	40	not required
Primavera	Lemon grass oil	00257A32	37974	40	not required
Taoasis	Lemon grass oil	130930-116754	31549	60	not required
Taoasis	Lemon grass oil	19425	38599	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 7 reference samples from the substance/substance group *Lemon grass oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 7 different batches.
- 27 634 spectra from a total of 593 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Bombastus	Lemon grass oil	294338	33012	40
Bombastus	Lemon grass oil	22002451	36885	40
Primavera	Lemon grass oil	00536M26	34370	40
Taoasis	Lemon grass oil	1448-127048	32977	40

- 30 770 spectra from a total of 705 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 38 spectra from 19 *Apo-Ident* customers from 32 batches from the substance/substance group *Lemon grass oil*.
- Among them are spectra of independent samples from 31 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Lemon grass oil	22000100	1
All	Lemon grass oil	23001197	1
Bombastus	Lemon grass oil	17001236	1
Bombastus	Lemon grass oil	20003469	1
Bombastus	Lemon grass oil	201215-20	1
Bombastus	Lemon grass oil	270423	1
Bombastus	Lemon grass oil	308065	1
Caelo	Lemon grass oil	17004202	1
Caelo	Lemon grass oil	504H26	2
Primavera, Gehe	Lemon grass oil	52A28	1
Primavera, Gehe	Lemon grass oil	61E28	2
Primavera, Gehe	Lemon grass oil	833B27	1
Primavera	Lemon grass oil	11401144	1
primavera	Lemon grass oil	279E31	1
Primavera	Lemon grass oil	516L31	1
Primavera	Lemon grass oil	52A28	1
Primavera	Lemon grass oil	61E28	1
Primavera/Sanacorp	Lemon grass oil	484A25	1
Taoasis	Lemon grass oil	104373-11249	1
Taoasis	Lemon grass oil	113127-12707	1
Taoasis	Lemon grass oil	130930-115336	1
Taoasis	Lemon grass oil	13131-112982	1
Taoasis	Lemon grass oil	1448-126624	1
Taoasis	Lemon grass oil	1448-128742	1
Taoasis	Lemon grass oil	1448-507	1
Taoasis	Lemon grass oil	1663-125423	1
Taoasis	Lemon grass oil	17004202	1
Taoasis	Lemon grass oil	1777-2776	1
Taoasis	Lemon grass oil	18988-125876	1
Taoasis	Lemon grass oil	2020113127-13387	2
Taoasis	Lemon grass oil	532897-111140	1
Taoasis	Lemon grass oil	6093-6119	1
Taoasis	Lemon grass oil	8911011-121890	1
Taoasis	Lemon grass oil	FFL457-123568	1
Taoasis	Lemon grass oil	L4A186361-10246	1

- 20 740 spectra from 1559 *Apo-Ident* customers from a total of 6320 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	300	0	27 634
Type B	0	160	0	30 770
Type C	0	38	0	20 740

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9615 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.0595 %)	100.0000 % (> 84.2105 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30661	30661	0.00	30.30
31185	31185	0.00	38.53
31187	31187	0.00	35.48
31549	31549	0.00	31.70
36040	36040	0.00	33.02
37974	37974	0.00	31.76
38599	38599	0.00	35.86

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Mandarin oil, green**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 33798-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Mandarin oil, green

Special notes

When selecting the *Mandarin oil, green* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Mandarin oil, green	2	2	2

Second-stage model

For differentiation of the substance/substance group *Mandarin oil, green* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mandarin oil, green* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citric oil	24.82	—
Lime oil	28.96	—
Grapefruit oil, organic	41.58	—
Orange oil	52.60	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Mandarin oil, green*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Mandarin oil, green	00431E25	33798	40	not required
Primavera	Mandarin oil, green	00381H25	33806	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Mandarin oil, green*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 2 different batches.
- 27 854 spectra from a total of 598 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are

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

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Mandarin oil, green	00425M25	33960	40
Primavera	Mandarin oil, green	00350J26	34397	40

- 30 850 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Mandarin oil, green*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis	Mandarin oil, green	110776-2806	1
Taoasis	Mandarin oil, green	2020102885-11907	1

- 20 776 spectra from 1559 *Apo-Ident* customers from a total of 6350 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	80	0	27 854
Type B	0	80	0	30 850
Type C	0	2	0	20 776

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9623 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0834 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33798	33798	0.00	24.60
33806	33806	0.00	25.02

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Manuka oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31545-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Manuka oil; Oleum leptospermum scoparium

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Manuka oil	5	2	13

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Manuka oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Vetiver bourbon oil	13.33	—
Immortelle oil	23.84	—
Lemon grass oil	28.81	—
Cypress oil	32.93	—
Myrtle oil	33.29	—
Citrus oil	38.06	—
Marjoram oil	40.44	—
Cedar wood oil	45.37	—
Cumin oil	46.13	—
Hyssop oil	46.14	—
Cardamom oil	46.83	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Manuka oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Manuka oil	1235-116650	31545	60	not required
Taoasis	Manuka oil	14286-119821	31655	60	not required
Taoasis	Manuka oil	83579-2408	33994	40	not required
Taoasis	Manuka oil	5181-9263	35075	40	not required
Taoasis	Manuka oil	11561-17382	37797	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Manuka oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 694 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 3 reference samples from the substance/substance group *Manuka oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Manuka oil	00476A27	34390	40
Taoasis	Manuka oil	42798-125299	32799	40
Taoasis	Manuka oil	42798-125299	33198	40

- 30 810 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 35 spectra from 7 *Apo-Ident* customers from 17 batches from the substance/substance group *Manuka oil*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Manuka oil		10
	Manuka oil	155G25	1
Canea Pharma GmbH	Manuka oil		1
Primavera	Manuka oil	899C28	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Taoasis	Manuka oil	23694-122415	1
Taoasis	Manuka oil	23694-123569	1
Taoasis	Manuka oil	2501-3536	1
Taoasis	Manuka oil	36968-121509	1
Taoasis	Manuka oil	42798-125299	3
Taoasis	Manuka oil	42798-126332	2
Taoasis	Manuka oil	5181-9263	1
Taoasis	Manuka oil	5191-13012	3
Taoasis	Manuka oil	65261-127051	1
Taoasis	Manuka oil	83579-2220	4
Taoasis	Manuka oil	96134-2223	1
Taoasis	Manuka oil	96134-2927	3

- 20 743 spectra from 1559 *Apo-Ident* customers from a total of 6335 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	240	0	27 694
Type B	0	120	0	30 810
Type C	0	35	0	20 743

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0596 %)	100.0000 % (> 82.8571 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31545	31545	0.00	37.15
31655	31655	0.00	36.53
33994	33994	0.00	27.29
35075	35075	0.00	23.08
37797	37797	0.00	23.31

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Marjoram oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30454-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Marjoram oil; Majoranae aetheroleum

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Marjoram oil	7	2	28

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Marjoram oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Tea tree oil	19.44	—
Carrot seed oil	28.64	—
Patchouli oil	54.57	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Marjoram oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Marjoram oil	16170005	32819	40	not required
Caelo	Marjoram oil	190992	34436	40	20190410*
Caelo	Marjoram oil	22001760003	36741	40	not required
Taoasis	Marjoram oil	130312-111991BAG90451	31137	40	not required
Taoasis	Marjoram oil	3701004-121123	32067	60	not required
Taoasis	Marjoram oil	1700187-3444	34275	40	not required
Taoasis	Marjoram oil	2022110211-16558	37665	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

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

Type A All calibration spectra.

- 300 spectra of 7 reference samples from the substance/substance group *Marjoram oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 7 different batches.
- 27 634 spectra from a total of 593 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 3 reference samples from the substance/substance group *Marjoram oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Marjoram oil	20004432007	36583	40
Taoasis	Marjoram oil	1838-125624	32478	40
Caelo	Marjoram oil	16170005	32919	40

- 30 810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 42 spectra from 15 *Apo-Ident* customers from 29 batches from the substance/substance group *Marjoram oil*.
- Among them are spectra of independent samples from 28 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Marjoram oil	115592	1
	Marjoram oil	2022110211-16558	1
Bombastus	Marjoram oil	278279	1
Caelo	Marjoram oil	12041602	7

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continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Marjoram oil	13041601	1
Caelo	Marjoram oil	13041603	2
Caelo	Marjoram oil	13041606	1
Caelo	Marjoram oil	13121301	1
Caelo	Marjoram oil	14198304	1
Caelo	Marjoram oil	14198305	1
Caelo	Marjoram oil	15051505	1
Caelo	Marjoram oil	18028305	1
Caelo	Marjoram oil	22001760004	1
Taoasis	Marjoram oil	115592-13308	1
Taoasis	Marjoram oil	115592-14822	1
Taoasis	Marjoram oil	11592-13308	1
Taoasis	Marjoram oil	11938-9221	1
Taoasis	Marjoram oil	130312-111347	1
Taoasis	Marjoram oil	130312-111870	1
Taoasis	Marjoram oil	130910-116960	1
Taoasis	Marjoram oil	130910-117430	1
Taoasis	Marjoram oil	1631-122347	1
Taoasis	Marjoram oil	1631-124621	1
Taoasis	Marjoram oil	1801859-7282	1
Taoasis	Marjoram oil	1838-127470	3
Taoasis	Marjoram oil	1987-1387	3
Taoasis	Marjoram oil	1987-767	1
Taoasis	Marjoram oil	29293-98717	1
Taoasis	Marjoram oil	3701004-119994	2
Taoasis/Gehe	Marjoram oil	29293-98717	1

- 20 736 spectra from 1559 *Apo-Ident* customers from a total of 6323 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	300	0	27 634
Type B	0	120	0	30 810
Type C	0	42	0	20 736

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9615 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0594 %)	100.0000 % (> 85.7143 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31137	31137	0.00	66.32
32067	32067	0.00	42.27
32819	32819	0.00	53.34
34275	34275	0.00	54.59
34436	34436	0.00	46.29
36741	36741	0.00	44.13
37665	37665	0.00	72.26

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group	Matricaria oil, morrocan
Substance class	BR APIs & excipients, liquid/semi-solid (other)
Report date	28/04/2026
Report number	30844-2026-04-28
Executing company	HiperScan GmbH Gerokstraße 13 01307 Dresden Germany

Relevant substance names

Matricaria oil, morrocan; Oleum ormenis multicaulis

Special notes

When selecting the *Matricaria oil, morrocan* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Matricaria oil, morrocan	4	3	9

Second-stage model

For differentiation of the substance/substance group *Matricaria oil, morrocan* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Matricaria oil, morrocan* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Camphor oil	32.96	—
Thyme oil, white	33.08	—
Marjoram oil	41.17	—
Citus oil	41.88	—
Angelica root oil	44.47	—
Yarrow oil	51.78	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Matricaria oil, morrocan*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Matricaria oil, morrocan	140124-116959	31579	60	not required
Taoasis	Matricaria oil, morrocan	6121017-122184	31841	60	not required
Taoasis	Matricaria oil, morrocan	1629-124596	32269	40	not required
Taoasis	Matricaria oil, morrocan	7111-16811	37663	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 4 reference samples from the substance/substance group *Matricaria oil, morrocan*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.

- 27734 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Matricaria oil, morrocan	6982-1074109BAC90451	30844	40
Taoasis	Matricaria oil, morrocan	1629-125295	32480	40
Taoasis	Matricaria oil, morrocan	1814-126707	33020	40

- 30810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 11 spectra from 5 *Apo-Ident* customers from 9 batches from the substance/substance group *Matricaria oil, morrocan*.
- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis	Matricaria oil, morrocan	5081-11906	1
Taoasis	Matricaria oil, morrocan	6159-93239	1
Taoasis	Matricaria oil, morrocan	6631-104465	1
Taoasis	Matricaria oil, morrocan	7111-12881	2
Taoasis	Matricaria oil, morrocan	7111-14502	2
Taoasis	Matricaria oil, morrocan	711114502	1
Taoasis/Taoasis	Matricaria oil, morrocan	1814-127407	1
Taoasis/Taoasis	Matricaria oil, morrocan	2022-960	1
Taoasis/Taoasis	Matricaria oil, morrocan	5081-8452	1

- 20 767 spectra from 1559 *Apo-Ident* customers from a total of 6343 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	120	0	30 810
Type C	0	10	1	20 767

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0628 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31579	31579	0.00	41.12
31841	31841	0.00	42.74
32269	32269	0.00	50.66
37663	37663	0.00	44.05

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

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Matricaria oil, roman**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31254-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Matricaria oil, roman

Special notes

When selecting the *Matricaria oil, roman* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Matricaria oil, roman	4	2	10

Second-stage model

For differentiation of the substance/substance group *Matricaria oil, roman* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Matricaria oil, roman* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sage oil	24.01	—
Citrus oil	29.85	—
Hyssop oil	32.79	—
Rosemary camphor oil	35.48	—
Spruce needle oil	37.51	—
Vetiver bourbon oil	37.76	—
Cedar wood oil	47.39	—
Rosemary oil	49.13	—
Cardamom oil	50.65	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Matricaria oil, roman*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Matricaria oil, roman	34561-112874	31254	40	not required
Taoasis	Matricaria oil, roman	1850119-119823	31686	60	not required
Taoasis	Matricaria oil, roman	2033-843	33989	40	not required
Taoasis	Matricaria oil, roman	111119-8815	35538	60	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 4 reference samples from the substance/substance group *Matricaria oil, roman*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27734 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 3 reference samples from the substance/substance group *Matricaria oil, roman*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Matricaria oil, roman	8941-125875	32796	40
Taoasis	Matricaria oil, roman	8841-15721	37649	40
Taoasis	Matricaria oil, roman	8941-125875	32978	40

- 30810 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 20 spectra from 2 *Apo-Ident* customers from 10 batches from the substance/substance group *Matricaria oil, roman*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Primavera	Matricaria oil, roman	579g27	1
Taoasis	Matricaria oil, roman	1511-122183	1
Taoasis	Matricaria oil, roman	1638-123706	1
Taoasis	Matricaria oil, roman	1850119-116753	1
Taoasis	Matricaria oil, roman	1850119-118138	1
Taoasis	Matricaria oil, roman	1850119-119451	1

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Supplier	Substance	Batch	Spectra
Taoasis	Matricaria oil, roman	1850119-121467	1
Taoasis	Matricaria oil, roman	1930-126600	7
Taoasis	Matricaria oil, roman	2033-3091	5
Taoasis	Matricaria oil, roman	8941-125875	1

- 20 758 spectra from 1559 *Apo-Ident* customers from a total of 6342 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	95	25	30 810
Type C	0	20	0	20 758

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9566 %)	79.1667 % (> 76.6667 %)
Type C	100.0000 % (> 99.0607 %)	100.0000 % (> 70.0000 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31254	31254	0.00	34.80
31686	31686	0.00	36.69
33989	33989	0.00	32.79
35538	35538	0.00	25.03

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Melissa oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 33800-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Melissa oil

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Melissa oil	5	1	0

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Melissa oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Immortelle oil	13.74	—
Lemon grass oil	15.04	—
Ginger oil	22.58	—
Vetiver bourbon oil	27.01	—
Cypress oil	27.84	—
Dwarf pine oil	28.75	—
Spearmint oil	30.46	—
Cedar wood oil	33.63	—
Marjoram oil	33.66	—
Citrus oil	34.60	—
Swiss pine oil	35.11	—
Citronella oil	39.24	—
Myrtle oil	39.67	—
Patchouli oil	44.41	—
Carrot seed oil	46.75	—
Tea tree oil	48.06	—
Manuka oil	49.06	—
Silver fir oil	51.48	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Melissa oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Melissa oil	00720H25	33800	40	not required
Primavera	Melissa oil	00065E26	34166	40	not required
Primavera	Melissa oil	00026A27	34404	40	not required
Taoasis	Melissa oil	640	33831	40	not required
Taoasis	Melissa oil	19400	38780	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Melissa oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 734 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Melissa oil	00010J26	34298	30

- 30 900 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Melissa oil*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 20 778 spectra from 1559 *Apo-Ident* customers from a total of 6352 batches from a further 167 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	30	0	30 900
Type C	0	0	0	20 778

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9573 %)	100.0000 % (> 80.0000 %)
Type C	100.0000 % (> 99.0752 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33800	33800	0.00	20.38
33831	33831	0.00	20.76
34166	34166	0.00	23.28
34404	34404	0.00	17.10
38780	38780	0.00	28.62

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

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Melissa oil 30%**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 33812-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Melissa oil 30%; Melissa 30% (essential oil)

Special notes

When selecting the *Melissa oil 30%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Melissa oil 30%	2	1	0

Second-stage model

For differentiation of the substance/substance group *Melissa oil 30%* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Melissa oil 30%* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, white	26.24	—
Petitgrain oil	26.86	—
Lavender oil	26.98	—
Neroli oil	27.27	—
Matricaria oil, morrocan	31.58	—
Bergamot oil	46.63	—
Yarrow oil	48.13	—
Spearmint oil	49.85	—
Juniper berry oil	50.77	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Melissa oil 30%* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Melissa oil 30%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Melissa oil 30%	01029J25	33812	40	not required
Primavera	Melissa oil 30%	00344A26	33962	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Melissa oil 30%*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 2

different batches.

- 27 854 spectra from a total of 598 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 30 spectra of 1 reference samples from the substance/substance group *Melissa oil 30%*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Melissa oil 30%	00362G26	34297	30

- 30 900 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Melissa oil 30%*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 20 778 spectra from 1559 *Apo-Ident* customers from a total of 6352 batches from a further 167 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Melissa oil 30%* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Melissa oil 30%* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following

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

	False positive	True positive	False negative	True negative
Type A	0	80	0	27 854
Type B	0	30	0	30 900
Type C	0	0	0	20 778

The substance/substance group *Melissa oil 30%* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9623 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9573 %)	100.0000 % (> 80.0000 %)
Type C	100.0000 % (> 99.0752 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33812	33812	0.00	26.86
33962	33962	0.00	27.25

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Myrrh oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30748-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Myrrh oil; Oleum myrrha

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Myrrh oil	6	2	4

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Myrrh oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Bergamot oil	36.65	—
Orange oil	47.87	—
Grapefruit oil, organic	50.44	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Myrrh oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Myrrh oil	00519L31	37978	40	not required
Taoasis	Myrrh oil	30007-120958	31692	60	not required
Taoasis	Myrrh oil	41197-124418BAG90451	32271	40	not required
Taoasis	Myrrh oil	2206-2428	33992	40	not required
Taoasis	Myrrh oil	9172-16661	37667	40	not required
Taoasis	Myrrh oil	20263	38782	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Myrrh oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 6 different batches.

- 27 674 spectra from a total of 594 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 120 spectra of 3 reference samples from the substance/substance group *Myrrh oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Myrrh oil	22920-105398BAG90451	30748	40
Taoasis	Myrrh oil	41197-126694	33050	40
Taoasis	Myrrh oil	41197-126694	33051	40

- 30 810 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 5 spectra from 2 *Apo-Ident* customers from 4 batches from the substance/substance group *Myrrh oil*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis	Myrrh oil	17F02206-4099	1
Taoasis	Myrrh oil	2067-107953	1
Taoasis	Myrrh oil	2206-1873	2
Taoasis	Myrrh oil	2379-6234	1

- 20 773 spectra from 1559 *Apo-Ident* customers from a total of 6348 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#),

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

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	260	0	27 674
Type B	0	80	40	30 810
Type C	0	5	0	20 773

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9566 %)	66.6667 % (> 64.1667 %)
Type C	100.0000 % (> 99.0683 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31692	31692	0.00	107.95
32271	32271	0.00	149.08
33992	33992	0.00	44.25
37667	37667	0.00	140.10
37978	37978	0.00	54.75
38782	38782	0.00	84.22

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Neroli oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31260-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Neroli oil; Oleum neroli

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Neroli oil	6	3	0

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Neroli oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, white	23.22	—
Matricaria oil, morrocan	25.86	—
Lavender oil	26.63	—
Basil oil	39.34	—
Melissa oil 30%	44.84	—
Coriander oil	50.74	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Neroli oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Neroli oil	00237B27	34406	40	not required
Primavera	Neroli oil	00123K31	37981	40	not required
Taoasis	Neroli oil	91029-115714	31260	40	not required
Taoasis	Neroli oil	6142-120057BAG90451	31695	60	not required
Taoasis	Neroli oil	0717/4-3018	34283	40	not required
Taoasis	Neroli oil	9001-16202	37668	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Neroli oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 6 different batches.
- 27 674 spectra from a total of 594 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 160 spectra of 4 reference samples from the substance/substance group *Neroli oil*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Neroli oil	00383G31	37789	40
Taoasis	Neroli oil	125052-124958	32805	40
Taoasis	Neroli oil	071704-1966	33993	40
Taoasis	Neroli oil	125052-124958	33042	40

- 30 770 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Neroli oil*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 20 778 spectra from 1559 *Apo-Ident* customers from a total of 6352 batches from a further 167 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	260	0	27 674
Type B	0	80	80	30 770
Type C	0	0	0	20 778

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9565 %)	50.0000 % (> 48.1250 %)
Type C	100.0000 % (> 99.0752 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31260	31260	0.00	48.32
31695	31695	0.00	51.87
34283	34283	0.00	55.78
34406	34406	0.00	41.03
37668	37668	0.00	39.34
37981	37981	0.00	65.88

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Nicotine**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31019-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Nicotine

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Nicotine	3	1	0

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nicotine* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dichloroacetic acid	147.03	–

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Nicotine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Roth	Nicotine	152183017	31019	20	1402687
Roth	Nicotine	194210173	31508	60	1410523
Roth	Nicotine	194210173	31518	60	not required
Roth	Nicotine	116210173	31948	45	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 185 spectra of 4 reference samples from the substance/substance group *Nicotine*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.
- 27 749 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by

this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Roth	Nicotine	137210173	33291	40

- 30 890 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Nicotine*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 20 778 spectra from 1559 *Apo-Ident* customers from a total of 6352 batches from a further 167 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	185	0	27 749
Type B	0	40	0	30 890
Type C	0	0	0	20 778

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 96.7568 %)
Type B	100.0000 % (> 99.9570 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.0752 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31019	31019	0.00	167.04
31508	31508	0.00	165.80
31518	31518	0.00	166.12
31948	31948	0.00	166.62

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Orange aroma**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31190-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Orange aroma; Orange flavour

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Orange aroma	7	9	122

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Orange aroma* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ethanol 70%	35.37	–

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Orange aroma*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Orange aroma	13123307	31190	40	not required
Caelo	Orange aroma	13406108	31402	40	not required
Caelo	Orange aroma	163470	33100	40	20161221*
Caelo	Orange aroma	20000419	35255	40	20200220*
Fagron	Orange aroma	13H23-B41-295530	31510	60	not required
Fagron	Orange aroma	18I17-B06-366492	35087	40	not required
Fagron	Orange aroma	23H09-T03-106056	38453	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

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

- 300 spectra of 7 reference samples from the substance/substance group *Orange aroma*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 7 different batches.
- 27 634 spectra from a total of 593 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Orange aroma	162063	32331	40
Caelo	Orange aroma	173005	33881	40
Caelo	Orange aroma	180831	34076	40
Caelo	Orange aroma	182057	34224	40
Caelo	Orange aroma	183261	34323	40
Caelo	Orange aroma	190933	34629	40
Caelo	Orange aroma	22001814006	36577	40
Caelo	Orange aroma	23000935	38139	40
Caelo	Orange aroma	24002146002	38942	40

- 30 570 spectra from a total of 700 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 830 spectra from 454 *Apo-Ident* customers from 126 batches from the substance/substance group *Orange aroma*.
- Among them are spectra of independent samples from 122 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Orange aroma	17300501	1
	Orange aroma	2002146006	1
	Orange aroma	220003369002	1
	Orange aroma	22000874008	3
	Orange aroma	22001814003	1
	Orange aroma	22001814005	1
	Orange aroma	22001814006	1
	Orange aroma	22001814008	1
	Orange aroma	22001814010	4
	Orange aroma	22001814011	5
	Orange aroma	22003359008	1
	Orange aroma	22003369002	4
	Orange aroma	22003369005	3
	Orange aroma	22003369006	1
	Orange aroma	22003369008	12
	Orange aroma	22003737003	15
	Orange aroma	22003737006	6
	Orange aroma	2203737003	1
	Orange aroma	2300035005	1
	Orange aroma	23000935004	1
	Orange aroma	23000935005	23
	Orange aroma	23003287004	11
	Orange aroma	24002146001	3
	Orange aroma	24002146002	36
	Orange aroma	24002146006	7
7,95	Orange aroma	22001814010	1
AHC	Orange aroma	23000935005	1
AHD	Orange aroma	23003287004	1
Allergika/Kehr	Orange aroma	16056107	1
Anzag	Orange aroma	22001814008	1
Anzag	Orange aroma	23000935005	1
Anzag	Orange aroma	250724 (24002146006)	1
Audor Pharma	Orange aroma	15215409	1
Bombastus	Orange aroma	21002295004	1
Cae	Orange aroma	20003349005	1
Caelo	Orange aroma		2
Caelo	Orange aroma	12216712	2
Caelo	Orange aroma	12356502	1
Caelo	Orange aroma	12356503	2
Caelo	Orange aroma	13123305	2
Caelo	Orange aroma	13123309	2
Caelo	Orange aroma	13330206	2
Caelo	Orange aroma	13330207	1
Caelo	Orange aroma	13406101	2
Caelo	Orange aroma	13406104	1
Caelo	Orange aroma	13406108	4
Caelo	Orange aroma	14150703	2
Caelo	Orange aroma	14150706	4
Caelo	Orange aroma	14150707	6
Caelo	Orange aroma	14150714	2
Caelo	Orange aroma	14352903	1
Caelo	Orange aroma	14352904	3
Caelo	Orange aroma	14352906	2
Caelo	Orange aroma	15215401	2
Caelo	Orange aroma	15215402	4
Caelo	Orange aroma	15215403	3
Caelo	Orange aroma	15215408	5
Caelo	Orange aroma	15215410	1
Caelo	Orange aroma	16056105	10
Caelo	Orange aroma	16056107	5

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Supplier	Substance	Batch	Spectra
Caelo	Orange aroma	16056108	1
Caelo	Orange aroma	160566107	1
Caelo	Orange aroma	16206301	3
Caelo	Orange aroma	16206302	1
Caelo	Orange aroma	16347005	12
Caelo	Orange aroma	16347012	3
Caelo	Orange aroma	17055103	3
Caelo	Orange aroma	17055104	2
Caelo	Orange aroma	17055110	1
Caelo	Orange aroma	17300501	12
Caelo	Orange aroma	17300507	11
Caelo	Orange aroma	17300508	1
Caelo	Orange aroma	17300509	7
Caelo	Orange aroma	180830103	1
Caelo	Orange aroma	18083103	11
Caelo	Orange aroma	18205701	18
Caelo	Orange aroma	18205702	2
Caelo	Orange aroma	18221702	1
Caelo	Orange aroma	18326103	31
Caelo	Orange aroma	18326104	1
Caelo	Orange aroma	18326108	8
Caelo	Orange aroma	18326113	10
Caelo	Orange aroma	1909312	1
Caelo	Orange aroma	19093301	13
Caelo	Orange aroma	19093302	2
Caelo	Orange aroma	19093307	7
Caelo	Orange aroma	19093309	1
Caelo	Orange aroma	19093311	13
Caelo	Orange aroma	19093312	4
Caelo	Orange aroma	192968003	16
Caelo	Orange aroma	192968005	4
Caelo	Orange aroma	200000419003	2
Caelo	Orange aroma	200000419004	1
Caelo	Orange aroma	20000419003	11
Caelo	Orange aroma	20000419006	18
Caelo	Orange aroma	20000419010	2
Caelo	Orange aroma	20000419012	9
Caelo	Orange aroma	20003349001	2
Caelo	Orange aroma	20003349002	9
Caelo	Orange aroma	20003349005	16
Caelo	Orange aroma	20003349008	2
Caelo	Orange aroma	20003349011	13
Caelo	Orange aroma	2000419003	1
Caelo	Orange aroma	2000419006	1
Caelo	Orange aroma	2003349002	1
Caelo	Orange aroma	21002295004	8
Caelo	Orange aroma	21002295009	2
Caelo	Orange aroma	21002295010	18
Caelo	Orange aroma	21002295013	14
Caelo	Orange aroma	210022955004	1
Caelo	Orange aroma	220000874003	1
Caelo	Orange aroma	22000874001	1
Caelo	Orange aroma	22000874003	13
Caelo	Orange aroma	22000874008	10
Caelo	Orange aroma	22001814003	7
Caelo	Orange aroma	22001814006	12
Caelo	Orange aroma	22001814008	7
Caelo	Orange aroma	22001814010	3
Caelo	Orange aroma	22003369008	1
Caelo	Orange aroma	22003737006	3

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Supplier	Substance	Batch	Spectra
Caelo	Orange aroma	2200874008	1
Caelo	Orange aroma	2201814008	1
Caelo	Orange aroma	2203369008	1
Caelo	Orange aroma	220905 (22000874003)	1
Caelo	Orange aroma	2300935005	1
Caelo	Orange aroma	23051201	1
Caelo	Orange aroma	24002146002	1
Caelo	Orange aroma	25031304	1
Caelo	Orange aroma	3(18326113)	1
Caelo	Orange aroma	4(20000419006)	1
Caelo	Orange aroma	7055210022954	1
Caelo	Orange aroma	92968005	1
Caesa / Alliance Hea...	Orange aroma	20003349011	1
Caesar & Loretz GmbH...	Orange aroma	22000874008	1
Caesar & Loretz GmbH...	Orange aroma	16347005	1
Caesar & Loretz GmbH...	Orange aroma	21002295004	1
Caesar & Loretz GmbH...	Orange aroma	22000874008	1
Caesar & Loretz GmbH...	Orange aroma	20003349005	1
Caesar & Loretz GmbH	Orange aroma	17300502	1
Caesar & Loretz GmbH	Orange aroma	17300509	1
Caesar & Loretz GmbH	Orange aroma	18083103	1
Caesar & Loretz GmbH	Orange aroma	18205701	2
Caesar & Loretz GmbH	Orange aroma	18326103	8
Caesar & Loretz GmbH	Orange aroma	18326113	4
Caesar & Loretz GmbH	Orange aroma	19093301	1
Caesar & Loretz GmbH	Orange aroma	19093302	1
Caesar & Loretz GmbH	Orange aroma	19093307	3
Caesar & Loretz GmbH	Orange aroma	19093311	6
Caesar & Loretz GmbH	Orange aroma	192968003	1
Caesar & Loretz GmbH	Orange aroma	192968007	1
Caesar & Loretz GmbH	Orange aroma	20000419003	12
Caesar & Loretz GmbH	Orange aroma	20000419006	4
Caesar & Loretz GmbH	Orange aroma	20000419007	2
Caesar & Loretz GmbH	Orange aroma	20000419012	8
Caesar & Loretz GmbH	Orange aroma	20003349001	3
Caesar & Loretz GmbH	Orange aroma	20003349002	3
Caesar & Loretz GmbH	Orange aroma	20003349005	4
Caesar & Loretz GmbH	Orange aroma	20003349011	5
Caesar & Loretz GmbH	Orange aroma	21002295004	5
Caesar & Loretz GmbH	Orange aroma	21002295009	1
Caesar & Loretz GmbH	Orange aroma	21002295010	9
Caesar & Loretz GmbH	Orange aroma	21002295013	4
Caesar & Loretz GmbH	Orange aroma	22000874003	4
Caesar & Loretz GmbH	Orange aroma	22000874008	5
Caesar & Loretz GmbH	Orange aroma	22001814002	1
Caesar & Loretz GmbH	Orange aroma	22001814003	1
Caesar & Loretz GmbH	Orange aroma	22001814006	4
Caesar & Loretz GmbH	Orange aroma	22001814008	3
Caesar & Loretz GmbH	Orange aroma	22001814010	1
Caesar & Loretz GmbH	Orange aroma	22001814011	1
Caesar & Loretz GmbH	Orange aroma	22003369002	2
Caesar & Loretz GmbH	Orange aroma	22003369008	1
Caesar & Loretz GmbH...	Orange aroma	20000419012	1
Caesar & Loretz GmbH...	Orange aroma	19093311	1
Caesar & Loretz GmbH...	Orange aroma	22001814011	1
Caesar & Loretz GmbH...	Orange aroma	22000874003	1
Caesar & Loretz GmbH...	Orange aroma	20003349011	1
Caesar & Loretz GmbH/AHD	Orange aroma	21002295004	1
Caesar & Loretz GmbH/AHD	Orange aroma	22000874003	1
Caesar & Loretz GmbH...	Orange aroma	20003349011	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/E	Orange aroma	22000874003	2
Caesar & Loretz GmbH/Gehe	Orange aroma	18205701	1
Caesar & Loretz GmbH/Gehe	Orange aroma	19093311	1
Caesar & Loretz GmbH/GEHE	Orange aroma	192968003	1
Caesar & Loretz GmbH/Gehe	Orange aroma	20003349005	1
Caesar & Loretz GmbH/Kehr	Orange aroma	18326103	1
Caesar & Loretz GmbH/Kehr	Orange aroma	20000419006	1
Caesar & Loretz GmbH...	Orange aroma	22000874003	2
Caesar & Loretz GmbH...	Orange aroma	21002295010	1
Caesar & Loretz GmbH...	Orange aroma	20000419003	1
Caesar & Loretz GmbH...	Orange aroma	20000419006	1
Caesar & Loretz GmbH...	Orange aroma	21002295010	1
Caesar & Loretz GmbH...	Orange aroma	22000874003	1
Caesar & Loretz GmbH...	Orange aroma	22003369008	1
Caesar & Loretz Hild...	Orange aroma	2003349002	1
Caesar & Loretz/Geil...	Orange aroma	18326103	1
Caesar & Loretz/Geil...	Orange aroma	20000419006	1
Caesar Loretz	Orange aroma	20000419006	1
Caesar&Lorenz	Orange aroma	21002295004	1
Caesar&Loretz GmbH/ ...	Orange aroma	17300501	1
Caesar&Loretz GmbH/ ...	Orange aroma	19093301	1
Euro OTC	Orange aroma	17055103	1
Fa.Phönix	Orange aroma	182050701	1
Fagron	Orange aroma	14352904	1
Fagron	Orange aroma	17300507	1
Fagron	Orange aroma	17A30-B02-335197	1
Fagron	Orange aroma	18I17-B06-366492	1
Gehe amax	Orange aroma	192968003	1
Gehe	Orange aroma	16056107	1
GEHE	Orange aroma	17300507	1
gehe	Orange aroma	18326103	1
Gehe	Orange aroma	18326108	1
Gehe	Orange aroma	20000419003	1
Gehe	Orange aroma	22001814008	1
Gehe	Orange aroma	22003369008	1
Gehe	Orange aroma	22003737006	1
Gehe	Orange aroma	23000935005	1
Geilenkirchen	Orange aroma	19093301	1
Henry LamotteOlis GmbH	Orange aroma	18205701	1
Holdermann	Orange aroma	23000935005	3
INTERN-DROGEN	Orange aroma	20003349005	1
Jenne	Orange aroma	240326(23000935005)	1
Nachprüfung	Orange aroma	19093311	1
Noweda	Orange aroma	18326103	1
Noweda	Orange aroma	20003349011	1
Noweda	Orange aroma	21002295004	1
Noweda	Orange aroma	22000874008	1
Noweda	Orange aroma	22001814003	1
Noweda	Orange aroma	22001814005	1
Noweda	Orange aroma	22001814010	2
Noweda	Orange aroma	2200874008	1
Noweda	Orange aroma	24002146002	1
Phoenix	Orange aroma	17300509	3
Phoenix	Orange aroma	18326103	2
Phoenix	Orange aroma	22001814011	1
Phoenix	Orange aroma	23000935005	1
Phoenix	Orange aroma	23003287004	1
Phönix 17.1.19	Orange aroma	18083103	1
Phönix	Orange aroma	18083103	1
Phönix	Orange aroma	22001814010	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Orange aroma	12356503	1
Sanacorp	Orange aroma	15387703	1
Sanacorp	Orange aroma	17300507	1
Sanacorp	Orange aroma	192968005	1
Sanacorp	Orange aroma	20003349005	1
Sanacorp	Orange aroma	23000935005	1
Sanacorp	Orange aroma	240021466006	1

- 19 948 spectra from 1528 *Apo-Ident* customers from a total of 6227 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	300	0	27 634
Type B	0	360	0	30 570
Type C	0	826	4	19 948

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9615 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9564 %)	100.0000 % (> 98.3333 %)
Type C	100.0000 % (> 99.0582 %)	99.5181 % (> 99.1566 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31190	31190	0.00	65.05
31402	31402	0.00	64.44
31510	31510	0.00	106.60
33100	33100	0.00	67.99
35087	35087	0.00	101.46
35255	35255	0.00	57.15
38453	38453	0.00	99.29

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Oregano oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31554-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Oregano oil; Oleum origani cretici

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Oregano oil	6	1	6

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Oregano oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, red	22.40	—
Savory herb	55.84	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Oregano oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Oregano oil	00256M26	34368	40	not required
Taoasis	Oregano oil	0131022-117999	31554	60	not required
Taoasis	Oregano oil	7921018-119483	31779	60	not required
Taoasis	Oregano oil	43878A-125814	32769	40	not required
Taoasis	Oregano oil	44314A-129096	33649	40	not required
Taoasis	Oregano oil	20298	38594	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 6 reference samples from the substance/substance group *Oregano oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 6 different batches.

- 27 654 spectra from a total of 594 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Oregano oil	43878A-123201	32939	40

- 30 890 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 7 spectra from 4 *Apo-Ident* customers from 6 batches from the substance/substance group *Oregano oil*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis	Oregano oil	B3010-11908	1
Taoasis	Oregano oil	B3010-13379	2
Taoasis	Oregano oil	B3253-15017	1
Taoasis/ Phönix	Oregano oil	44314A-1600	1
Taoasis/Gehe	Oregano oil	6553TR-L03	1
Taoasis/Noweda	Oregano oil	B3253-16203	1

- 20 771 spectra from 1559 *Apo-Ident* customers from a total of 6346 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#),

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

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	280	0	27 654
Type B	0	40	0	30 890
Type C	0	7	0	20 771

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9615 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9570 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.0654 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31554	31554	0.00	61.20
31779	31779	0.00	81.49
32769	32769	0.00	42.18
33649	33649	0.00	43.13
34368	34368	0.00	67.03
38594	38594	0.00	43.78

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Palmarosa oil, organic**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30597-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Palmarosa oil, organic; Oleum palmarosae

Special notes

When selecting the *Palmarosa oil, organic* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Palmarosa oil, organic	3	4	10

Second-stage model

For differentiation of the substance/substance group *Palmarosa oil, organic* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Palmarosa oil, organic* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Rose-geranium oil, organic	89.67	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Palmarosa oil, organic*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Palmarosa oil, organic	2461021-121891	31828	60	not required
Taoasis	Palmarosa oil, organic	4941003-126708	33043	40	not required
Taoasis	Palmarosa oil, organic	2141-3447	34289	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 3 reference samples from the substance/substance group *Palmarosa oil, organic*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.
- 27 794 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for

model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 240 spectra of 6 reference samples from the substance/substance group *Palmarosa oil, organic*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Palmarosa oil, organic	00500L26	34366	40
Taoasis	Palmarosa oil, organic	17524-105015BAG90451	30597	40
Taoasis	Palmarosa oil, organic	104704-129227	33856	40
Taoasis	Palmarosa oil, organic	19009	38595	40
Taoasis	Palmarosa oil, organic	17524-105015BAG90451	30671	40
Taoasis	Palmarosa oil, organic	4941003-126708	33044	40

- 30 690 spectra from a total of 704 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 12 spectra from 9 *Apo-Ident* customers from 10 batches from the substance/substance group *Palmarosa oil, organic*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Noweda	Palmarosa oil, organic	194F32	1
Primavera	Palmarosa oil, organic	724G27	1
Taoasis GmbH/ Taoasis	Palmarosa oil, organic	2587-7434	1
Taoasis	Palmarosa oil, organic	121018-111094	1
Taoasis	Palmarosa oil, organic	121018-111872	2
Taoasis	Palmarosa oil, organic	2242	1
Taoasis	Palmarosa oil, organic	2587-9089	1
Taoasis	Palmarosa oil, organic	5044-14506	1
Taoasis/Sanacorp/05...	Palmarosa oil, organic	18545044-12851	1
Taoasis/Taoasis	Palmarosa oil, organic	121018-111872	1
Taoasis/Taoasis	Palmarosa oil, organic	2215-5590	1

- 20 766 spectra from 1559 *Apo-Ident* customers from a total of 6342 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	140	0	27 794
Type B	0	240	0	30 690
Type C	0	11	1	20 766

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9618 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.0624 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31828	31828	0.00	108.55
33043	33043	0.00	96.28
34289	34289	0.00	103.20

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

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Patchouli oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31547-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Patchouli oil; Oleum pogostemon cablin

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Patchouli oil	4	4	2

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Patchouli oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	16.16	—
Lemon grass oil	18.91	—
Tea tree oil	23.18	—
Dwarf pine oil	31.14	—
Carrot seed oil	31.63	—
Melissa oil	36.65	—
Vetiver bourbon oil	36.79	—
Immortelle oil	37.46	—
Citronella oil	38.63	—
Cedar wood oil	40.56	—
Cypress oil	48.94	—
Rose-geranium oil, organic	57.97	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Patchouli oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Patchouli oil	14167204	31619	60	not required
Taoasis	Patchouli oil	130930-112789	31547	60	not required
Taoasis	Patchouli oil	FFL735-123003	32172	40	not required
Taoasis	Patchouli oil	108398-16513	37669	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 4 reference samples from the substance/substance group *Patchouli oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 734 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 200 spectra of 5 reference samples from the substance/substance group *Patchouli oil*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Patchouli oil	00475B27	34389	40
Primavera	Patchouli oil	00329A32	37976	40
Taoasis	Patchouli oil	1633-126207	33031	40
Taoasis	Patchouli oil	P29-1186	34113	40
Taoasis	Patchouli oil	1633-126207	33032	40

- 30 730 spectra from a total of 705 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 2 spectra from 1 *Apo-Ident* customers from 2 batches from the substance/substance group *Patchouli oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis	Patchouli oil	130930-116684	1
Taoasis	Patchouli oil	33474-119161	1

- 20 776 spectra from 1559 *Apo-Ident* customers from a total of 6350 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	101	99	30 730
Type C	0	2	0	20 776

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9565 %)	50.5000 % (> 49.0000 %)
Type C	100.0000 % (> 99.0834 %)	n/a (n/a)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31547	31547	0.00	28.08
31619	31619	0.00	33.06
32172	32172	0.00	33.92
37669	37669	0.00	39.51

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

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Peppermint oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30930-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Peppermint oil; Oleum menthae piperitae dopp. rectific.

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Peppermint oil	5	6	202

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Peppermint oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	56.63	–

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Peppermint oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Peppermint oil	00098J25	33809	40	not required
Primavera	Peppermint oil	00425G31	37785	40	not required
Taoasis	Peppermint oil	443428-83579	30930	40	not required
Taoasis	Peppermint oil	525728-109217B	30965	40	not required
Taoasis	Peppermint oil	2016104277-125426	32481	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Peppermint oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 734 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are

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

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

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Peppermint oil	00374B26	33958	40
Primavera	Peppermint oil	00221G26	34168	40
Primavera	Peppermint oil	00465A27	34371	40
Taoasis	Peppermint oil	2016104277-126375	32804	40
Taoasis	Peppermint oil	104277-126684	33030	40
Taoasis	Peppermint oil	219067-16604	37670	40

- 30 690 spectra from a total of 703 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 460 spectra from 339 *Apo-Ident* customers from 204 batches from the substance/substance group *Peppermint oil*.
- Among them are spectra of independent samples from 200 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Peppermint oil	1343122	1
	Peppermint oil	20003483015	1
	Peppermint oil	20264	1
	Peppermint oil	2200013001	1
	Peppermint oil	22000130016	4
	Peppermint oil	22000130024	4
	Peppermint oil	22000613006	1
	Peppermint oil	22002982001	1
	Peppermint oil	22002982004	1
	Peppermint oil	22002982006	3

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Supplier	Substance	Batch	Spectra
	Peppermint oil	22002982007	1
	Peppermint oil	22003829	2
	Peppermint oil	2207007-01	2
	Peppermint oil	22C09-T06-098222	1
	Peppermint oil	23000689	1
	Peppermint oil	23000983002	3
	Peppermint oil	23000983004	1
	Peppermint oil	23002616	1
	Peppermint oil	23003248001	12
	Peppermint oil	230032481	1
	Peppermint oil	23003687	2
	Peppermint oil	23006-T20-102556	1
	Peppermint oil	2305006-01	3
	Peppermint oil	23106-T02-106822	2
	Peppermint oil	23I-T02-106822	1
	Peppermint oil	23I06-T02-106822	1
	Peppermint oil	24000498001	2
	Peppermint oil	24001264008	1
	Peppermint oil	2400498001	1
	Peppermint oil	24H13-T01-115167	1
	Peppermint oil	25000838006	1
	Peppermint oil	76E32	1
AHD	Peppermint oil	22000130020	1
AHD	Peppermint oil	22000130024	1
AHD	Peppermint oil	23000983004	1
AHD	Peppermint oil	23003840	1
Alliance Healthcare	Peppermint oil	18006685	1
Alliance	Peppermint oil	22000130024	2
Alliance	Peppermint oil	22002982006	1
Alliance	Peppermint oil	24002894	1
Anzag	Peppermint oil	241017 (24002894)	1
Apotheke Bauer & Cie...	Peppermint oil		1
bambastus	Peppermint oil	21002270	1
Bombastus	Peppermint oil	20005390	1
Bombastus	Peppermint oil	18003695	2
Bombastus	Peppermint oil	18005114	3
Bombastus	Peppermint oil	180051143413	1
Bombastus	Peppermint oil	18006685	5
Bombastus	Peppermint oil	19001155	3
Bombastus	Peppermint oil	19004746	5
Bombastus	Peppermint oil	19005821	1
Bombastus	Peppermint oil	1900588	1
Bombastus	Peppermint oil	19005885	1
Bombastus	Peppermint oil	20001874	1
Bombastus	Peppermint oil	20001977	5
Bombastus	Peppermint oil	20003390	2
Bombastus	Peppermint oil	20004131	1
Bombastus	Peppermint oil	20004136	1
Bombastus	Peppermint oil	20005390	1
Bombastus	Peppermint oil	21004165	3
Bombastus	Peppermint oil	21004204	1
Bombastus	Peppermint oil	22000376	1
Bombastus	Peppermint oil	22000609	1
Bombastus	Peppermint oil	22003313	1
Bombastus	Peppermint oil	23003687	1
Bombastus	Peppermint oil	286204	1
Bombastus	Peppermint oil	303064	1
Bombastus	Peppermint oil	307854	4
Caelo	Peppermint oil	12114225	1
Caelo	Peppermint oil	1319I-01995	1

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Supplier	Substance	Batch	Spectra
Caelo	Peppermint oil	14369919	1
Caelo	Peppermint oil	15255818	1
Caelo	Peppermint oil	16114602	1
Caelo	Peppermint oil	16114611	1
Caelo	Peppermint oil	16114613	1
Caelo	Peppermint oil	16114625	1
Caelo	Peppermint oil	16114628	1
Caelo	Peppermint oil	16114630	1
Caelo	Peppermint oil	1703032-01	1
Caelo	Peppermint oil	17188609	3
Caelo	Peppermint oil	17188612	1
Caelo	Peppermint oil	17291901	1
Caelo	Peppermint oil	17340813	1
Caelo	Peppermint oil	17364301	1
Caelo	Peppermint oil	18000796	1
Caelo	Peppermint oil	18003695	1
Caelo	Peppermint oil	18009910	1
Caelo	Peppermint oil	18208401	3
Caelo	Peppermint oil	18208405	1
Caelo	Peppermint oil	18208412	1
Caelo	Peppermint oil	18221701	3
Caelo	Peppermint oil	18221702	9
Caelo	Peppermint oil	18221712	5
Caelo	Peppermint oil	18221715	1
Caelo	Peppermint oil	18221716	8
Caelo	Peppermint oil	18221719	1
Caelo	Peppermint oil	18221723	6
Caelo	Peppermint oil	18221725	1
Caelo	Peppermint oil	19000776001	1
Caelo	Peppermint oil	19000776010	1
Caelo	Peppermint oil	191136001	2
Caelo	Peppermint oil	19113601	1
Caelo	Peppermint oil	19113603	2
Caelo	Peppermint oil	191359004	2
Caelo	Peppermint oil	191359005	1
Caelo	Peppermint oil	191359006	1
Caelo	Peppermint oil	191359007	9
Caelo	Peppermint oil	19135902	1
Caelo	Peppermint oil	19135905	7
Caelo	Peppermint oil	19135908	1
Caelo	Peppermint oil	19139005	1
Caelo	Peppermint oil	200000648008	1
Caelo	Peppermint oil	20000648006	1
Caelo	Peppermint oil	20000648007	1
Caelo	Peppermint oil	20000648008	20
Caelo	Peppermint oil	20000648010	1
Caelo	Peppermint oil	20003483002	2
Caelo	Peppermint oil	20003483006	14
Caelo	Peppermint oil	20003483007	1
Caelo	Peppermint oil	20003483009	1
Caelo	Peppermint oil	20003483011	1
Caelo	Peppermint oil	20003483014	11
Caelo	Peppermint oil	20003483015	3
Caelo	Peppermint oil	20003589001	2
Caelo	Peppermint oil	2000358901	1
Caelo	Peppermint oil	20003795002	3
Caelo	Peppermint oil	20003795005	3
Caelo	Peppermint oil	20003795008	3
Caelo	Peppermint oil	20003795010	1
Caelo	Peppermint oil	20003991003	3

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Supplier	Substance	Batch	Spectra
Caelo	Peppermint oil	2000648008	1
Caelo	Peppermint oil	2003483014	1
Caelo	Peppermint oil	2003795005	1
Caelo	Peppermint oil	22000130001	1
Caelo	Peppermint oil	22000130003	7
Caelo	Peppermint oil	22000130008	5
Caelo	Peppermint oil	22000130016	2
Caelo	Peppermint oil	22000130020	1
Caelo	Peppermint oil	22000130022	1
Caelo	Peppermint oil	22000130024	1
Caelo	Peppermint oil	220001303	1
Caelo	Peppermint oil	22000613006	4
Caelo	Peppermint oil	22002982001	4
Caelo	Peppermint oil	22002982006	1
Caelo	Peppermint oil	220282001	1
Caelo	Peppermint oil	617Q-01995	1
Caelo	Peppermint oil	9135901	1
Caelo	Peppermint oil	W474	1
Caesar & Loretz GmbH...	Peppermint oil	22000130003	1
Caesar & Loretz GmbH...	Peppermint oil	22000130008	1
Caesar & Loretz GmbH	Peppermint oil	191359004	1
Caesar & Loretz GmbH	Peppermint oil	20000648008	3
Caesar & Loretz GmbH	Peppermint oil	20003483006	1
Caesar & Loretz GmbH	Peppermint oil	20003483010	1
Caesar & Loretz GmbH	Peppermint oil	20003483014	4
Caesar & Loretz GmbH	Peppermint oil	20003991003	1
Caesar & Loretz GmbH	Peppermint oil	2003483014	1
Caesar & Loretz GmbH	Peppermint oil	22000130003	1
Caesar & Loretz GmbH	Peppermint oil	22000130010	1
Caesar & Loretz GmbH...	Peppermint oil	20003795010	1
Caesar und Loretz	Peppermint oil	20003795005	1
caesar	Peppermint oil	24000498001	1
Caesar&Loretz GmbH	Peppermint oil	20003483006	1
EuRho	Peppermint oil	2011012-02	1
Euro OTC	Peppermint oil	1231489	1
Euro OTC	Peppermint oil	16114611	1
Euro OTC	Peppermint oil	1804008-01	1
Euro OTC	Peppermint oil	1804008-02	3
Euro OTC	Peppermint oil	180400802	1
Euro OTC	Peppermint oil	19005885	1
Euro OTC	Peppermint oil	2011012-01	1
Euro OTC	Peppermint oil	2011012-22	1
Euro OTC	Peppermint oil	201101201	1
Fagron	Peppermint oil	1142326	1
Fagron	Peppermint oil	15B11-B08-304117	1
Fagron	Peppermint oil	18B08-B06	1
Fagron	Peppermint oil	19C14-B12-191227	3
Fagron	Peppermint oil	19C14-B14-191227	1
Fagron	Peppermint oil	19F01-803	1
Fagron	Peppermint oil	19j21-b14-193446	1
Fagron	Peppermint oil	19J21-B14-193446	1
Fagron	Peppermint oil	20A14-B01-197082	2
Fagron	Peppermint oil	20C16-B07-201867	5
Fagron	Peppermint oil	21/17-T08-090070	2
Fagron	Peppermint oil	21117-T06-093899	1
Fagron	Peppermint oil	21E12-086267	1
Fagron	Peppermint oil	21E12-TQ2-088277	1
Fagron	Peppermint oil	21I17-T08-093899	2
Fagron	Peppermint oil	22H09-T06-099349	1
Fagron	Peppermint oil	23C06-T20-102556	1

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Supplier	Substance	Batch	Spectra
Fagron	Peppermint oil	8-09007000	1
Gehe	Peppermint oil	17F08-B07-339333	1
Gehe	Peppermint oil	1800796	1
Gehe	Peppermint oil	18221716	1
Gehe	Peppermint oil	20003483014	1
Gehe	Peppermint oil	22000130020	1
Gehe	Peppermint oil	2200130016	1
Gehe	Peppermint oil	23003248001	1
Gehe	Peppermint oil	23C06-T20-102556	2
Gehe	Peppermint oil	24H13-T01-1151	1
Gehe	Peppermint oil	24H13-T01-115167	1
Hänseler	Peppermint oil		1
Jenne	Peppermint oil	230418(21004165)	1
jenne	Peppermint oil	24000498001	1
Kehr	Peppermint oil	22000130024	1
Kögl	Peppermint oil	421211154615	1
Melsan	Peppermint oil	1705811	1
Noweda	Peppermint oil	1900776010	1
Noweda	Peppermint oil	20000648008	1
Noweda	Peppermint oil	21117-T08-093899	1
Noweda	Peppermint oil	21M7-T08-093899	1
Noweda	Peppermint oil	22000130020	1
noweda	Peppermint oil	22000130024	1
Noweda	Peppermint oil	22000130024	3
Noweda	Peppermint oil	22002982001	1
Noweda	Peppermint oil	22002982007	1
Noweda	Peppermint oil	2207007-01	2
Noweda	Peppermint oil	22H09-T06-099349	1
Noweda	Peppermint oil	23003687	1
Noweda	Peppermint oil	24001264008/2506110	1
Ph/Euro	Peppermint oil	170303202	1
Phoenix 28.12..18	Peppermint oil	18221702	1
Phoenix	Peppermint oil	19135905	1
Phoenix	Peppermint oil	22000130024	1
Phoenix	Peppermint oil	24000498001	1
Phönix	Peppermint oil	22000130016	1
Phönix	Peppermint oil	22000376	1
Phönix	Peppermint oil	24000498001	1
Primavera, Gehe	Peppermint oil	762G25	1
Primavera	Peppermint oil	191K27	1
Primavera	Peppermint oil	291C29	1
Primavera	Peppermint oil	61M27	1
Primavera/AHD	Peppermint oil	13112017	1
sanacorp	Peppermint oil	23000983002	1
sanacorp	Peppermint oil	24000498001	1
Sanacorp	Peppermint oil	24002894	1
Taoasis	Peppermint oil	111455-6397	3
Taoasis	Peppermint oil	123108-7608	1
Taoasis	Peppermint oil	165305-13915	2
Taoasis	Peppermint oil	1800141-3963	1
Taoasis	Peppermint oil	24699-117643	1
Taoasis	Peppermint oil	40076-120885	1
Taoasis	Peppermint oil	41798-121607	1
Taoasis	Peppermint oil	52216-123564	1
Taoasis	Peppermint oil	63561-125104	1
Taoasis	Peppermint oil	63561-125729	1
Taoasis	Peppermint oil	63561-126008	2
Taoasis	Peppermint oil	65074-125102BAG90451	1
Taoasis	Peppermint oil	75404-127882	1
Taoasis	Peppermint oil	78725-128653	1

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Supplier	Substance	Batch	Spectra
Taoasis	Peppermint oil	79725-12653	1
Taoasis	Peppermint oil	79725-126853	1
Taoasis	Peppermint oil	79725-128653	2
Taoasis	Peppermint oil	88914-2568	1
Taoasis	Peppermint oil	93360-3339	4
Taoasis/ Kehr	Peppermint oil	41798-120746H08	1
Taoasis/Kehr	Peppermint oil	127711	1
TAOASIS/phönix	Peppermint oil	7308L09-CN	1
Taoasis/Taoasis	Peppermint oil	167107-15033	1
Taoasis/Taoasis	Peppermint oil	41798-12517	1
Toasis/Noweda	Peppermint oil		2

- 20 318 spectra from 1523 *Apo-Ident* customers from a total of 6150 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	222	18	30 690
Type C	0	446	14	20 318

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9565 %)	92.5000 % (> 91.2500 %)
Type C	100.0000 % (> 99.0583 %)	96.9565 % (> 96.3043 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30930	30930	0.00	73.17
30965	30965	0.00	75.64
32481	32481	0.00	64.55
33809	33809	0.00	60.92
37785	37785	0.00	63.38

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Raspberry aroma**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30562-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Raspberry aroma; Raspberry flavour

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Raspberry aroma	5	8	129

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Raspberry aroma* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Strawberry aroma	36.21	–
Contramarum aroma	52.44	–

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Raspberry aroma*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Raspberry aroma	12246612	31171	40	1402588
Caelo	Raspberry aroma	14115902	31396	40	not required
Caelo	Raspberry aroma	16126605	33222	40	not required
Caelo	Raspberry aroma	21002129009	36049	40	20210702
Caelo	Raspberry aroma	22000122006	36737	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Raspberry aroma*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 734 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this

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

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

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

- 320 spectra of 8 reference samples from the substance/substance group *Raspberry aroma*.
- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Raspberry aroma	12054307	30611	40
Caelo	Raspberry aroma	15438503	33054	40
Caelo	Raspberry aroma	172581	33697	40
Caelo	Raspberry aroma	192776	34746	40
Caelo	Raspberry aroma	22003420	38131	40
Caelo	Raspberry aroma	23000538	38132	40
Caelo	Raspberry aroma	24002133	38908	40
Caelo	Raspberry aroma	24002904	38918	40

- 30610 spectra from a total of 701 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 669 spectra from 348 *Apo-Ident* customers from 134 batches from the substance/substance group *Raspberry aroma*.
- Among them are spectra of independent samples from 129 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Raspberry aroma	22002419003	1
	Raspberry aroma	22003420001	2
	Raspberry aroma	22003420006	1
	Raspberry aroma	22003420010	5
	Raspberry aroma	22003420011	4
	Raspberry aroma	22003420012	2
	Raspberry aroma	22003420016	10

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Supplier	Substance	Batch	Spectra
	Raspberry aroma	22003420018	2
	Raspberry aroma	2203420010	1
	Raspberry aroma	2203420016	1
	Raspberry aroma	23000538001	10
	Raspberry aroma	23000538003	1
	Raspberry aroma	23000538005	11
	Raspberry aroma	23000538006	1
	Raspberry aroma	231013(23000538001)	1
	Raspberry aroma	24001333002	16
	Raspberry aroma	24002133003	23
	Raspberry aroma	24002904002	2
Anzag06.	Raspberry aroma	14376109	1
Bombastus	Raspberry aroma	12246608	1
Caelo	Raspberry aroma	11303813	1
Caelo	Raspberry aroma	12054302	1
Caelo	Raspberry aroma	12054310	1
Caelo	Raspberry aroma	12054311	1
Caelo	Raspberry aroma	12246604	1
Caelo	Raspberry aroma	12246608	2
Caelo	Raspberry aroma	12246612	1
Caelo	Raspberry aroma	12246616	2
Caelo	Raspberry aroma	12246617	1
Caelo	Raspberry aroma	13255502	2
Caelo	Raspberry aroma	13255507	2
Caelo	Raspberry aroma	13255510	1
Caelo	Raspberry aroma	13255514	2
Caelo	Raspberry aroma	14115902	1
Caelo	Raspberry aroma	14115909	1
Caelo	Raspberry aroma	14115912	1
Caelo	Raspberry aroma	14115913	2
Caelo	Raspberry aroma	14376103	2
Caelo	Raspberry aroma	14376109	4
Caelo	Raspberry aroma	14376115	6
Caelo	Raspberry aroma	15219102	3
Caelo	Raspberry aroma	1521911	1
Caelo	Raspberry aroma	15219111	4
Caelo	Raspberry aroma	15438501	11
Caelo	Raspberry aroma	15438503	8
Caelo	Raspberry aroma	15438504	1
Caelo	Raspberry aroma	16126602	3
Caelo	Raspberry aroma	16126605	8
Caelo	Raspberry aroma	16126606	2
Caelo	Raspberry aroma	16126609	6
Caelo	Raspberry aroma	16126611	3
Caelo	Raspberry aroma	171872002	1
Caelo	Raspberry aroma	17187201	1
Caelo	Raspberry aroma	17187202	4
Caelo	Raspberry aroma	17187205	8
Caelo	Raspberry aroma	17187209	6
Caelo	Raspberry aroma	17187212	12
Caelo	Raspberry aroma	17187213	1
Caelo	Raspberry aroma	17258101	9
Caelo	Raspberry aroma	17258102	5
Caelo	Raspberry aroma	17258103	1
Caelo	Raspberry aroma	17258106	10
Caelo	Raspberry aroma	17258107	3
Caelo	Raspberry aroma	18074302	9
Caelo	Raspberry aroma	18074305	1
Caelo	Raspberry aroma	18074307	15
Caelo	Raspberry aroma	180743307	1

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Supplier	Substance	Batch	Spectra
Caelo	Raspberry aroma	18249905	2
Caelo	Raspberry aroma	18249907	3
Caelo	Raspberry aroma	18249910	3
Caelo	Raspberry aroma	18249911	1
Caelo	Raspberry aroma	18249912	2
Caelo	Raspberry aroma	191600002	1
Caelo	Raspberry aroma	19160001	7
Caelo	Raspberry aroma	19160002	23
Caelo	Raspberry aroma	19160006	9
Caelo	Raspberry aroma	1916006	1
Caelo	Raspberry aroma	192776	2
Caelo	Raspberry aroma	192776001	3
Caelo	Raspberry aroma	192776002	1
Caelo	Raspberry aroma	192776005	1
Caelo	Raspberry aroma	192776006	13
Caelo	Raspberry aroma	192776007	1
Caelo	Raspberry aroma	192776008	1
Caelo	Raspberry aroma	192776009	1
Caelo	Raspberry aroma	192776010	5
Caelo	Raspberry aroma	20002006001	1
Caelo	Raspberry aroma	20002006002	1
Caelo	Raspberry aroma	20002006003	17
Caelo	Raspberry aroma	20002006006	6
Caelo	Raspberry aroma	210000063011	1
Caelo	Raspberry aroma	21000063004	11
Caelo	Raspberry aroma	21000063005	1
Caelo	Raspberry aroma	21000063008	7
Caelo	Raspberry aroma	2100063011	1
Caelo	Raspberry aroma	21002109001	1
Caelo	Raspberry aroma	21002129001	5
Caelo	Raspberry aroma	21002129002	2
Caelo	Raspberry aroma	21002129006	9
Caelo	Raspberry aroma	21002129009	2
Caelo	Raspberry aroma	21002129011	5
Caelo	Raspberry aroma	2100219001	1
Caelo	Raspberry aroma	2100219006	1
Caelo	Raspberry aroma	2100219010	1
Caelo	Raspberry aroma	2100219011	1
Caelo	Raspberry aroma	2102129006	1
Caelo	Raspberry aroma	210512-05	1
Caelo	Raspberry aroma	217258101	1
Caelo	Raspberry aroma	22000122002	8
Caelo	Raspberry aroma	22000122006	10
Caelo	Raspberry aroma	22000122008	1
Caelo	Raspberry aroma	22000122009	1
Caelo	Raspberry aroma	22000122010	3
Caelo	Raspberry aroma	22000122011	8
Caelo	Raspberry aroma	22000122013	4
Caelo	Raspberry aroma	2200122009	1
Caelo	Raspberry aroma	22002419002	2
Caelo	Raspberry aroma	22002419003	9
Caelo	Raspberry aroma	22002419004	1
Caelo	Raspberry aroma	22002419006	4
Caelo	Raspberry aroma	22003420001	3
Caelo	Raspberry aroma	22003420002	2
Caelo	Raspberry aroma	22003420004	1
Caelo	Raspberry aroma	22003420005	2
Caelo	Raspberry aroma	2200342001	1
Caelo	Raspberry aroma	22003420010	4
Caelo	Raspberry aroma	22003420012	1

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Supplier	Substance	Batch	Spectra
Caelo	Raspberry aroma	22003420016	3
Caelo	Raspberry aroma	220808(22000122006)	1
Caeolo	Raspberry aroma	14376103	1
Caesar & Lorenz	Raspberry aroma	22003420001	1
Caesar & Loretz GmbH...	Raspberry aroma	21000063004	1
Caesar & Loretz GmbH...	Raspberry aroma	192776006	1
Caesar & Loretz GmbH...	Raspberry aroma	18249907	1
Caesar & Loretz GmbH...	Raspberry aroma	22002419003	1
Caesar & Loretz GmbH...	Raspberry aroma	22002419003	1
Caesar & Loretz GmbH...	Raspberry aroma	22003420011	1
Caesar & Loretz GmbH...	Raspberry aroma	192776006	1
Caesar & Loretz GmbH	Raspberry aroma	18074307	2
Caesar & Loretz GmbH	Raspberry aroma	18249905	1
Caesar & Loretz GmbH	Raspberry aroma	18249907	1
Caesar & Loretz GmbH	Raspberry aroma	18249910	3
Caesar & Loretz GmbH	Raspberry aroma	18249911	1
Caesar & Loretz GmbH	Raspberry aroma	18249912	3
Caesar & Loretz GmbH	Raspberry aroma	19160001	1
Caesar & Loretz GmbH	Raspberry aroma	19160002	13
Caesar & Loretz GmbH	Raspberry aroma	19160006	2
Caesar & Loretz GmbH	Raspberry aroma	19160008	1
Caesar & Loretz GmbH	Raspberry aroma	192776001	1
Caesar & Loretz GmbH	Raspberry aroma	192776006	6
Caesar & Loretz GmbH	Raspberry aroma	192776010	1
Caesar & Loretz GmbH	Raspberry aroma	20002006002	1
Caesar & Loretz GmbH	Raspberry aroma	20002006003	9
Caesar & Loretz GmbH	Raspberry aroma	20002006006	1
Caesar & Loretz GmbH	Raspberry aroma	21000063004	6
Caesar & Loretz GmbH	Raspberry aroma	21000063008	8
Caesar & Loretz GmbH	Raspberry aroma	2100212006	1
Caesar & Loretz GmbH	Raspberry aroma	21002129001	1
Caesar & Loretz GmbH	Raspberry aroma	21002129006	2
Caesar & Loretz GmbH	Raspberry aroma	21002129009	1
Caesar & Loretz GmbH	Raspberry aroma	21002129010	1
Caesar & Loretz GmbH	Raspberry aroma	22000122002	4
Caesar & Loretz GmbH	Raspberry aroma	22000122005	1
Caesar & Loretz GmbH	Raspberry aroma	22000122006	5
Caesar & Loretz GmbH	Raspberry aroma	22000122009	4
Caesar & Loretz GmbH	Raspberry aroma	22000122011	2
Caesar & Loretz GmbH	Raspberry aroma	22000122012	1
Caesar & Loretz GmbH	Raspberry aroma	22002419002	3
Caesar & Loretz GmbH	Raspberry aroma	22002419003	4
Caesar & Loretz GmbH	Raspberry aroma	22002419006	1
Caesar & Loretz GmbH	Raspberry aroma	22003420001	4
Caesar & Loretz GmbH	Raspberry aroma	22003420005	2
Caesar & Loretz GmbH	Raspberry aroma	22003420010	1
Caesar & Loretz GmbH/ AHD	Raspberry aroma	19160002	1
Caesar & Loretz GmbH...	Raspberry aroma	20002006006	1
Caesar & Loretz GmbH...	Raspberry aroma	18249902	1
Caesar & Loretz GmbH...	Raspberry aroma	22003420010	1
Caesar & Loretz GmbH/AHD	Raspberry aroma	22000122002	1
Caesar & Loretz GmbH...	Raspberry aroma	19160001	1
Caesar & Loretz GmbH...	Raspberry aroma	22000122011	1
Caesar & Loretz GmbH...	Raspberry aroma	22003420001	1
Caesar & Loretz GmbH/sana	Raspberry aroma	192776001	1
Caesar & Loretz GmbH...	Raspberry aroma	19160001	1
Caesar & Loretz GmbH...	Raspberry aroma	192776010	1
Caesar & Loretz GmbH...	Raspberry aroma	20002006003	1
Caesar & Loretz GmbH...	Raspberry aroma	21000063008	1
Caesar & Loretz GmbH...	Raspberry aroma	22000122012	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz Hilden	Raspberry aroma	19160002	1
Caesar & Loretz Hild...	Raspberry aroma	19160006	1
Caesar Loretz	Raspberry aroma	20002006003	1
Caesar/Noweda	Raspberry aroma	212m-07020	1
Caleo/Noveda	Raspberry aroma	21000063004	3
Fagron	Raspberry aroma	18074307	1
Fiebig	Raspberry aroma	17258106	1
Fiebig	Raspberry aroma	192776006	1
Gehe	Raspberry aroma	19160002	1
Gehe	Raspberry aroma	20002006003	1
Gehe	Raspberry aroma	21000063008	1
Gehe	Raspberry aroma	21002129009	1
Gehe	Raspberry aroma	22003420016	1
Gehe	Raspberry aroma	23000538005	1
Gehe	Raspberry aroma	2300058001	1
Gehe	Raspberry aroma	24001333002	1
Gehe	Raspberry aroma	24002133003	1
Henry Lamotte/AHD	Raspberry aroma	17538106	1
Intern Drogen/Phoenix	Raspberry aroma	15438501	1
INTERN-DROGEN	Raspberry aroma	21002129006	1
Kehr	Raspberry aroma	16126609	1
Kehr	Raspberry aroma	17187209	1
Kehr	Raspberry aroma	23000538001	1
Noveda	Raspberry aroma	210000063008	1
Noweda	Raspberry aroma	14115909	1
Noweda	Raspberry aroma	17258101	1
Noweda	Raspberry aroma	18249905	1
Noweda	Raspberry aroma	20002006003	1
NOWEDA	Raspberry aroma	22002419006	1
Noweda	Raspberry aroma	22003420005	1
Noweda	Raspberry aroma	23000538005	1
Noweda/ Caesar&Loren...	Raspberry aroma	192776001	1
Phoenix	Raspberry aroma	17258106	1
Phoenix	Raspberry aroma	18249910	1
Phoenix	Raspberry aroma	23000538005	1
Phönix Gotha	Raspberry aroma	12246612	1
Phönix	Raspberry aroma	15438506	1
Phönix	Raspberry aroma	18249905	1
Phönix	Raspberry aroma	20002006003	1
Phönix	Raspberry aroma	21002129006	1
Phönix	Raspberry aroma	24001333002	1
Rondell Apotheke	Raspberry aroma	15438501	1
Sanacorp	Raspberry aroma	19160002	1
Sanacorp	Raspberry aroma	22000122002	1
Sanacorp	Raspberry aroma	22002419005	1
Sanacorp	Raspberry aroma	22003420016	2
Sanacorp	Raspberry aroma	23000538001	1
Sanacorp	Raspberry aroma	23000538005	1
Sanacorp	Raspberry aroma	24002133003	1

- 20 109 spectra from 1528 *Apo-Ident* customers from a total of 6218 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	320	0	30 610
Type C	0	667	2	20 109

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9564 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.0583 %)	99.7010 % (> 99.2526 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31171	31171	0.00	61.45
31396	31396	0.00	65.37
33222	33222	0.00	70.81
36049	36737	5.70	52.49
36737	36737	0.00	54.56

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Ravintsara oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30386-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Ravintsara oil; Ravintsara (essentiell oil)

Special notes

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

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Ravintsara oil	3	3	15

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ravintsara oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Hyssop oil	13.10	—
Sage oil	17.60	—
Rosemary oil	23.15	—
Marjoram oil	25.13	—
Citrus oil	25.23	—
Myrtle oil	27.69	—
Rosemary camphor oil	33.31	—
Angelica root oil	33.66	—
Yarrow oil	35.20	—
Cypress oil	35.63	—
Niaouli oil	39.41	—
Matricaria oil, roman	41.06	—
Eucalyptus oil	41.71	—
Cajeput (essentielle oil)	47.82	—
Camphor oil	51.89	—

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Ravintsara oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Ravintsara oil	231012-118739	31635	60	not required
Taoasis	Ravintsara oil	1687-966	33854	40	not required
Taoasis	Ravintsara oil	1687-966	33872	40	not required
Taoasis	Ravintsara oil	20366	38603	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Ravintsara oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.
- 27 754 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 160 spectra of 4 reference samples from the substance/substance group *Ravintsara oil*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Ravintsara oil	00065B27	34403	40
Taoasis	Ravintsara oil	1687-125316	32803	40
Taoasis	Ravintsara oil	1994-3103	34285	40
Taoasis	Ravintsara oil	1687-125316	33029	40

- 30 770 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

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

- 21 spectra from 2 *Apo-Ident* customers from 16 batches from the substance/substance group *Ravintsara oil*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ravintsara oil	43L32	1
Taoasis	Ravintsara oil	1687-125316	1
Taoasis	Ravintsara oil	1687-126824	1
Taoasis	Ravintsara oil	1687-127661	1
Taoasis	Ravintsara oil	1944-1388	1
Taoasis	Ravintsara oil	1944-1733	1
Taoasis	Ravintsara oil	1994-3103	1
Taoasis	Ravintsara oil	2101005-116830	3
Taoasis	Ravintsara oil	231012-118738	1
Taoasis	Ravintsara oil	231012-118739	2
Taoasis	Ravintsara oil	231012-118892	1
Taoasis	Ravintsara oil	231012-119831	1
Taoasis	Ravintsara oil	231012-120291	1
Taoasis	Ravintsara oil	2427-5280	1
Taoasis	Ravintsara oil	59/144/17	1
Taoasis	Ravintsara oil	9331006-121650	3

- 20 757 spectra from 1559 *Apo-Ident* customers from a total of 6336 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	180	0	27 754
Type B	0	160	0	30 770
Type C	0	21	0	20 757

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.0606 %)	100.0000 % (> 71.4286 %)

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

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31635	31635	0.00	20.46
33854	33854	0.00	20.30
33872	33872	0.00	20.19
38603	38603	0.00	28.46

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

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Rose oil, pure**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 34034-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Rose oil, pure; Rose, pure (essential oil)

Special notes

When selecting the *Rose oil, pure* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Rose oil, pure	2	2	0

Second-stage model

For differentiation of the substance/substance group *Rose oil, pure* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Rose oil, pure* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Palmarosa oil, organic	50.59	–

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

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Rose oil, pure*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Rose oil, pure	00165C31	37790	40	not required
Taoasis	Rose oil, pure	12014-120330H08	34034	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Rose oil, pure*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 2 different batches.
- 27 854 spectra from a total of 598 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for

model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 80 spectra of 2 reference samples from the substance/substance group *Rose oil, pure*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Rose oil, pure	00099L26	34405	40
Primavera	Rose oil, pure	00647J31	37980	40

- 30 850 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Rose oil, pure*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 20 778 spectra from 1559 *Apo-Ident* customers from a total of 6352 batches from a further 167 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Rose oil, pure* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Rose oil, pure* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	80	0	27 854
Type B	0	40	40	30 850
Type C	0	0	0	20 778

The substance/substance group *Rose oil, pure* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9623 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9567 %)	50.0000 % (> 46.2500 %)
Type C	100.0000 % (> 99.0752 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
34034	34034	0.00	58.41
37790	37790	0.00	97.67

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group	Rose-geranium oil, organic
Substance class	BR APIs & excipients, liquid/semi-solid (other)
Report date	28/04/2026
Report number	30536-2026-04-28
Executing company	HiperScan GmbH Gerokstraße 13 01307 Dresden Germany

Relevant substance names

Rose-geranium oil, organic; Oleum pelargonium graveolens

Special notes

When selecting the *Rose-geranium oil, organic* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Rose-geranium oil, organic	4	2	33

Second-stage model

For differentiation of the substance/substance group *Rose-geranium oil, organic* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Rose-geranium oil, organic* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citronella oil	24.76	—
Carrot seed oil	46.08	—
Lemon grass oil	47.04	—
Marjoram oil	47.07	—
Vetiver bourbon oil	50.72	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Rose-geranium oil, organic* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Rose-geranium oil, organic*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Rose-geranium oil, organic	21027-119997	31698	60	not required
Taoasis	Rose-geranium oil, organic	21027-121893	31776	60	not required
Taoasis	Rose-geranium oil, organic	21027-121893	31951	60	not required
Taoasis	Rose-geranium oil, organic	1616008-125056	33036	40	not required
Taoasis	Rose-geranium oil, organic	19494	38591	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 5 reference samples from the substance/substance group *Rose-geranium oil, organic*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.

- 27674 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Rose-geranium oil, organic*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Rose-geranium oil, organic	00492L26	34372	40
Taoasis	Rose-geranium oil, organic	2260-2430	34042	40
Taoasis	Rose-geranium oil, organic	1616008-125056	33037	40

- 30810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 39 spectra from 15 *Apo-Ident* customers from 33 batches from the substance/substance group *Rose-geranium oil, organic*.
- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Rose-geranium oil, organic	19003MQS04	1
apomix	Rose-geranium oil, organic	2260-2431	1
Biofrid	Rose-geranium oil, organic	5010	1
Bombastus	Rose-geranium oil, organic	22625-106677	1
primavera	Rose-geranium oil, organic	177G27	1
Primavera	Rose-geranium oil, organic	8304131	1
Primavera/Primavera	Rose-geranium oil, organic	618L23	1
Primvera	Rose-geranium oil, organic	259E31	1
Taoasis	Rose-geranium oil, organic	130111-110467	1

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Supplier	Substance	Batch	Spectra
Taoasis	Rose-geranium oil, organic	130111-112615	1
Taoasis	Rose-geranium oil, organic	130729-113060	1
Taoasis	Rose-geranium oil, organic	1500969-123554	1
Taoasis	Rose-geranium oil, organic	1840-128860	2
Taoasis	Rose-geranium oil, organic	1840-374	2
Taoasis	Rose-geranium oil, organic	21027-119121	1
Taoasis	Rose-geranium oil, organic	21027-120292	1
Taoasis	Rose-geranium oil, organic	21027-121337	1
Taoasis	Rose-geranium oil, organic	2445-3346	1
Taoasis	Rose-geranium oil, organic	2445-3947	3
Taoasis	Rose-geranium oil, organic	2445-6615	1
Taoasis	Rose-geranium oil, organic	2520-7998	1
Taoasis	Rose-geranium oil, organic	401011-117641	1
Taoasis	Rose-geranium oil, organic	401011-117806	2
Taoasis	Rose-geranium oil, organic	4502-11389	1
Taoasis	Rose-geranium oil, organic	4502-9228	1
Taoasis	Rose-geranium oil, organic	6311-13014	1
Taoasis	Rose-geranium oil, organic	8341-1229	1
Taoasis	Rose-geranium oil, organic	8341-12299	1
Taoasis	Rose-geranium oil, organic	A1616008-128497	1
Taoasis/Taoasis	Rose-geranium oil, organic	2260-2430	1
Taoasis/Taoasis	Rose-geranium oil, organic	22625-104463	1
Taoasis/Taoasis	Rose-geranium oil, organic	2445-5861	1
Taoasis/Taoasis	Rose-geranium oil, organic	4502-9228	1
Taoasis/Taoasis	Rose-geranium oil, organic	B1840-128497	1

- 20 739 spectra from 1559 *Apo-Ident* customers from a total of 6319 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Rose-geranium oil, organic* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Rose-geranium oil, organic* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	27 674
Type B	0	120	0	30 810
Type C	0	39	0	20 739

The substance/substance group *Rose-geranium oil, organic* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0595 %)	100.0000 % (> 84.6154 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31698	31698	0.00	33.60
31776	31776	0.00	34.37
31951	31951	0.00	34.08
33036	33036	0.00	27.35
38591	38591	0.00	22.74

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Rosemary camphor oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 33803-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Rosemary camphor oil

Special notes

When selecting the *Rosemary camphor oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Rosemary camphor oil	4	2	2

Second-stage model

For differentiation of the substance/substance group *Rosemary camphor oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Rosemary camphor oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Rosemary oil	10.28	—
Citus oil	14.85	—
Hyssop oil	18.23	—
Eucalyptus oil	25.19	—
Ravintsara oil	25.74	—
Myrtle oil	29.23	—
Niaouli oil	31.90	—
Sage oil	32.15	—
Marjoram oil	35.12	—
Spruce needle oil	36.40	—
Cajeput (essentiel oil)	40.03	—
Cypress oil	41.90	—
Angelica root oil	45.65	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Rosemary camphor oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Rosemary camphor oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Rosemary camphor oil	00536K25	33803	40	not required
Primavera	Rosemary camphor oil	00559B26	33959	40	not required
Primavera	Rosemary camphor oil	00746D29	35733	30	20210916*
Primavera	Rosemary camphor oil	00473G28	35734	40	20210916*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 150 spectra of 4 reference samples from the substance/substance group *Rosemary camphor oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 784 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Rosemary camphor oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Rosemary camphor oil	00179G26	34170	40
Primavera	Rosemary camphor oil	00631A27	34373	40

- 30 850 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Rosemary camphor oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Primavera	Rosemary camphor oil	794L27	1
Primavera/Primavera	Rosemary camphor oil	21B29	1

- 20 776 spectra from 1559 *Apo-Ident* customers from a total of 6350 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Rosemary camphor oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Rosemary camphor oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	150	0	27 784
Type B	0	80	0	30 850
Type C	0	2	0	20 776

The substance/substance group *Rosemary camphor oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9618 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0834 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33803	33803	0.00	20.02
33959	33959	0.00	19.60
35733	35733	0.00	18.50
35734	35734	0.00	18.62

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Rosewood oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31556-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Rosewood oil; Oleum aniba roseodora

Special notes

When selecting the *Rosewood oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Rosewood oil	4	2	16

Second-stage model

For differentiation of the substance/substance group *Rosewood oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Rosewood oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, white	44.48	—
Coriander oil	68.73	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Rosewood oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Rosewood oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Rosewood oil	11572-116545	31556	60	not required
Taoasis	Rosewood oil	4381004-120355	31688	60	not required
Taoasis	Rosewood oil	42543-2657	34106	40	not required
Taoasis	Rosewood oil	19011	38590	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 4 reference samples from the substance/substance group *Rosewood oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 734 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are

listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Rosewood oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Rosewood oil	00632H26	34381	40
Taoasis	Rosewood oil	5101015-124967	32801	40
Taoasis	Rosewood oil	5101015-124967	33048	40

- 30810 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 31 spectra from 3 *Apo-Ident* customers from 16 batches from the substance/substance group *Rosewood oil*.
- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis GmbH/ Taoasis	Rosewood oil	109177-5788	1
Taoasis	Rosewood oil	109177-5788	4
Taoasis	Rosewood oil	42543-126343	1
Taoasis	Rosewood oil	42543-127664	1
Taoasis	Rosewood oil	42543-128055	2
Taoasis	Rosewood oil	42543-128666	1
Taoasis	Rosewood oil	42543-146	4
Taoasis	Rosewood oil	42543-2053	2
Taoasis	Rosewood oil	4381004-1200355	1
Taoasis	Rosewood oil	4381004-121143	2
Taoasis	Rosewood oil	4381004-122041	2
Taoasis	Rosewood oil	5101015-123299	1
Taoasis	Rosewood oil	5101015-124243	1

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Supplier	Substance	Batch	Spectra
Taoasis	Rosewood oil	5101015-124967	3
Taoasis	Rosewood oil	5101017-122566	2
Taoasis	Rosewood oil	9177-3983	2
Taoasis/Taoasis	Rosewood oil	109177-5863	1

- 20 747 spectra from 1559 *Apo-Ident* customers from a total of 6336 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Rosewood oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Rosewood oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	120	0	30 770
Type C	0	31	0	20 747

The substance/substance group *Rosewood oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9570 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0598 %)	100.0000 % (> 80.6452 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31556	31556	0.00	47.47
31688	31688	0.00	52.68
34106	34106	0.00	39.98
38590	38590	0.00	60.92

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Sage oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31139-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Sage oil; Oleum salviae

Special notes

When selecting the *Sage oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sage oil	4	1	21

Second-stage model

For differentiation of the substance/substance group *Sage oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sage oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Rosemary camphor oil	17.92	—
Spruce needle oil	22.94	—
Hyssop oil	24.29	—
Rosemary oil	28.39	—
Ravintsara oil	33.50	—
Eucalyptus oil	34.35	—
Matricaria oil, roman	36.20	—
Citrus oil	46.42	—
Marjoram oil	48.02	—
Camphor oil	51.87	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sage oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Sage oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Sage oil	526975-112642BAG90451	31139	40	not required
Taoasis	Sage oil	34052-114939	31257	40	not required
Taoasis	Sage oil	8461016-122272	31783	60	not required
Taoasis	Sage oil	L14121DN-17062	37672	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Sage oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 754 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Sage oil*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Sage oil	8461016-126496	33034	40
Taoasis	Sage oil	8461016-126496	33035	40

- 30 850 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 28 spectra from 14 *Apo-Ident* customers from 21 batches from the substance/substance group *Sage oil*.
- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Anzag	Sage oil	16451ITP11	1
	Sage oil	24000773002	1
	Sage oil	C42827	1
	Sage oil	240805(22003209008)	1
	Sage oil	18004276	2
	Sage oil	20004247	2
	Sage oil	22001659	1

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Supplier	Substance	Batch	Spectra
Bombastus	Sage oil	309857	1
Taoasis	Sage oil	13988-117449	1
Taoasis	Sage oil	21190-118009	1
Taoasis	Sage oil	21190-119239	1
Taoasis	Sage oil	29944-120889	1
Taoasis	Sage oil	29944-120965	1
Taoasis	Sage oil	461016-6429	2
Taoasis	Sage oil	8461016-127221	1
Taoasis	Sage oil	8461016-2158	1
Taoasis	Sage oil	8461016-3526	2
Taoasis	Sage oil	8461016-774	2
Taoasis	Sage oil	L14121DN-15434	1
Taoasis	Sage oil	L15820DN-13382	2
Taoasis/ Phoenix (28...	Sage oil	7156ITL06	1
Taoasis/Phoenix/22.0...	Sage oil	7156ITL06	1

- 20 750 spectra from 1559 *Apo-Ident* customers from a total of 6332 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Sage oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sage oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	180	0	27 754
Type B	0	80	0	30 850
Type C	0	28	0	20 750

The substance/substance group *Sage oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0600 %)	100.0000 % (> 78.5714 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31139	31139	0.00	36.77
31257	31257	0.00	34.14
31783	31783	0.00	22.94
37672	37672	0.00	38.28

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Sandalwood oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 33799-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Sandalwood oil

Special notes

When selecting the *Sandalwood oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sandalwood oil	4	3	2

Second-stage model

For differentiation of the substance/substance group *Sandalwood oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sandalwood oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Rose oil, pure	81.53	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sandalwood oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Sandalwood oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Sandalwood oil	00891G25	33799	40	not required
Primavera	Sandalwood oil	00141L25	33801	40	not required
Taoasis	Sandalwood oil	145-505	33832	40	not required
Taoasis	Sandalwood oil	18165	38597	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Sandalwood oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 774 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by

this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Sandalwood oil*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Sandalwood oil	00474C26	34173	40
Primavera	Sandalwood oil	00346L26	34408	40
Taoasis	Sandalwood oil	128319	33833	40

- 30810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 1 *Apo-Ident* customers from 2 batches from the substance/substance group *Sandalwood oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Primavera	Sandalwood oil	703G27	1
Taoasis	Sandalwood oil	9791-14508	3

- 20774 spectra from 1559 *Apo-Ident* customers from a total of 6350 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Sandalwood oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sandalwood oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	160	0	27 774
Type B	0	120	0	30 810
Type C	0	4	0	20 774

The substance/substance group *Sandalwood oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9618 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9566 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.0708 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33799	33799	0.00	90.31
33801	33801	0.00	93.77
33832	33832	0.00	81.53
38597	38597	0.00	103.05

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Savory herb**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 33820-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Savory herb

Special notes

When selecting the *Savory herb* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Savory herb	3	1	3

Second-stage model

For differentiation of the substance/substance group *Savory herb* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Savory herb* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, red	23.67	—
Oregano oil	24.83	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Savory herb* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Savory herb*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Savory herb	498	33820	40	not required
Taoasis	Savory herb	1569-129318	33821	40	not required
Taoasis	Savory herb	19833	38772	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Savory herb*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.
- 27 814 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by

this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Savory herb*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Savory herb	1742-3729	34281	40

- 30 890 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Savory herb*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis / Sanacorp	Savory herb	6514-15397	1
Taoasis	Savory herb	6003ESL07	1
Taoasis	Savory herb	6514-13875	2

- 20 774 spectra from 1559 *Apo-Ident* customers from a total of 6349 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Savory herb* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose,

all relevant spectra of the various substances were compared with *Savory herb* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	120	0	27 814
Type B	0	40	0	30 890
Type C	0	4	0	20 774

The substance/substance group *Savory herb* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9619 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9570 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.0708 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33820	33820	0.00	25.31
33821	33821	0.00	23.67
38772	38772	0.00	29.09

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Sebexol®/Wofacutan/Hans Karrer/Excipial**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 10006709-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Sebexol®/Wofacutan/Hans Karrer/Excipial; Amciderm® Base cream; Excipial® U Hydrolotio; Hans Karrer Hydrocream MicroSilver; Nourivan™ Antiox; Sebexol® basic pH 5 formula basis; Sebexol® cream lotion; Wofacutan wash lotion

Special notes

When selecting the *Sebexol®/Wofacutan/Hans Karrer/Excipial* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sebexol®/Wofacutan/Hans Karrer/Excipial	29	14	328

Second-stage model

For differentiation of the substance/substance group *Sebexol®/Wofacutan/Hans Karrer/Excipial* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sebexol®/Wofacutan/Hans Karrer/Excipial* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dimeticono ointment 10% SR	17.54	—
Abitima® clinic face cream	21.41	—
Milk Cordes® O/W Emulsion	22.92	—
Base cream Taoasis	24.56	—
Hans Karrer Lipocream MicroSilver	32.09	—
ALLERGIKA® – Face cream MED	34.43	—
SyrSpend® SF pH4 cherry aroma	34.71	—
Hans Karrer Lipolotion MicroSilver	34.79	—
Neuroderm® care lotion	36.03	—
Asche Basis® lotion	36.10	—
Neuroderm® moisturising cream	36.31	—
Fabitop® base cream	36.87	—
Excipial® U10 Lipolotio	37.35	—
DMS® base cream classic	38.18	—
SyrSpend® SF pH4 aroma free	40.10	—
Aloe vera gel, 10x concentrated	40.41	—
Retterspitz external	42.66	—
DMS® base cream high classic	44.33	—
Water	46.42	—
Dexeryl®	48.20	—
Neribas® cream	51.00	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sebexol®/Wofacutan/Hans Karrer/Excipial* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Sebexol®/Wofacutan/Hans Karrer/Excipial*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Almirall	Amciderm [®] Base cream	313311	31509	60	not required
Almirall	Amciderm [®] Base cream	313311	31628	75	not required
Almirall	Amciderm [®] Base cream	650341	33502	40	not required
Almirall	Amciderm [®] Base cream	048171	36764	40	not required
Galderma L...	Excipial [®] U Hydrolotio	331554	35469	40	not required
Galderma L...	Excipial [®] U Hydrolotio	365111	36768	40	not required
Spirig Pharma	Excipial [®] U Hydrolotio	M016	30731	40	not required
Spirig Pharma	Excipial [®] U Hydrolotio	M063	31073	40	not required
Spirig Pharma	Excipial [®] U Hydrolotio	N013	31279	40	not required
Spirig Pharma	Excipial [®] U Hydrolotio	R014	31536	60	not required
Hans Karre...	Hans Karrer Hydrocream Mi...	16001	33190	40	not required
Hans Karre...	Hans Karrer Hydrocream Mi...	16002	33191	40	not required
Hans Karre...	Hans Karrer Hydrocream Mi...	18002	34116	40	not required
Hans Karre...	Hans Karrer Hydrocream Mi...	22004	36726	40	not required
Hans Karre...	Hans Karrer Hydrocream Mi...	22002	36727	40	not required
Fagron	Nourivan [™] Antiox	14C11-T09-010959	31495	60	not required
Fagron	Nourivan [™] Antiox	1503258	31958	45	not required
Fagron	Nourivan [™] Antiox	1703842	33789	30	not required
Devesa	Sebexol [®] basic pH 5 formu...	1307	31104	40	1403098
Devesa	Sebexol [®] basic pH 5 formu...	1522	31961	60	not required
Devesa	Sebexol [®] basic pH 5 formu...	1638124	32744	40	not required
Devesa	Sebexol [®] cream lotion	1220	30839	40	1403097
Devesa	Sebexol [®] cream lotion	1317	31103	40	not required
Devesa	Sebexol [®] cream lotion	1412	31592	45	not required
Devesa	Sebexol [®] cream lotion	1531	31839	60	not required
Devesa	Sebexol [®] cream lotion	1552.2	32743	40	not required
Devesa	Sebexol [®] cream lotion	2128114	36773	40	not required
Kesla Pharma	Wofacutan wash lotion	0974.12	30972	80	not required
Kesla Pharma	Wofacutan wash lotion	0389.13	31065	40	not required
Kesla Pharma	Wofacutan wash lotion	0868.16	33483	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1375 spectra of 30 reference samples from the substance/substance group *Sebexol[®]/Wofacutan/Hans Karrer/Excipial*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 29 different batches.
- 26 559 spectra from a total of 573 batches from further 137 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples:

In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 755 spectra of 20 reference samples from the substance/substance group *Sebexol®/Wofacutan/Hans Karrer/Excipial*.
- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Almirall	Amciderm® Base cream	538331	32758	40
Almirall	Amciderm® Base cream	822351	34365	40
Spirig Pharma	Excipial® U Hydrolotio	S061	33206	40
Spirig Pharma	Excipial® U Hydrolotio	V052	33981	40
Hans Karrer GmbH	Hans Karrer Hydrocream Mi...	16003	33192	40
Hans Karrer GmbH	Hans Karrer Hydrocream Mi...	16004	33193	40
Hans Karrer GmbH	Hans Karrer Hydrocream Mi...	21003	35574	50
Devesa	Sebexol® basic pH 5 formu...	1712122	33427	40
Devesa	Sebexol® basic pH 5 formu...	1644102	33432	40
Devesa	Sebexol® basic pH 5 formu...	2243126	37424	40
Devesa	Sebexol® cream lotion	1605101	32907	40
Devesa	Sebexol® cream lotion	2338120	38243	40
Kesla Pharma	Wofacutan wash lotion	0729.16	32913	40
Kesla Pharma	Wofacutan wash lotion	0061.22	36772	40
Fagron	Nourivan™ Antiox	1503258	31958 [†]	15
Fagron	Nourivan™ Antiox	1503258	32778	40
Fagron	Nourivan™ Antiox	1503258	32822	40
Fagron	Nourivan™ Antiox	1703842	33789 [†]	10
Devesa	Sebexol® cream lotion	1605101	32908	40
Kesla Pharma	Wofacutan wash lotion	0729.16	32914	40

- 30175 spectra from a total of 693 batches from further 204 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1945 spectra from 304 *Apo-Ident* customers from 330 batches from the substance/substance group *Sebexol®/Wofacutan/Hans Karrer/Excipial*.
- Among them are spectra of independent samples from 287 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sebexol® basic pH 5 formu...		4
	Amciderm® Base cream	212181	1
	Sebexol® cream lotion	2127208	1
	Sebexol® cream lotion	2149108	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Sebexol [®] cream lotion	2149110	2
	Hans Karrer Hydrocream Mi...	22006	1
	Sebexol [®] cream lotion	2243128	3
	Hans Karrer Hydrocream Mi...	23001	1
	Hans Karrer Hydrocream Mi...	23002	1
	Hans Karrer Hydrocream Mi...	23003	2
	Hans Karrer Hydrocream Mi...	23004	2
	Sebexol [®] cream lotion	2304125	4
	Sebexol [®] cream lotion	2304126	11
	Sebexol [®] basic pH 5 formu...	2316117	3
	Sebexol [®] cream lotion	2316118	8
	Sebexol [®] cream lotion	2316119	11
	Sebexol [®] cream lotion	2337114	15
	Sebexol [®] cream lotion	2338120	12
	Hans Karrer Hydrocream Mi...	24003	5
	Hans Karrer Hydrocream Mi...	24004	4
	Hans Karrer Hydrocream Mi...	24005	1
	Sebexol [®] cream lotion	241410	1
	Sebexol [®] cream lotion	2414102	5
	Sebexol [®] cream lotion	2414103	25
	Sebexol [®] cream lotion	2414402	1
	Sebexol [®] basic pH 5 formu...	2427103	12
	Sebexol [®] cream lotion	2436105	6
	Sebexol [®] cream lotion	2436106	6
	Sebexol [®] cream lotion	2436109	1
	Sebexol [®] cream lotion	2513124	2
	Sebexol [®] cream lotion	2513224	1
	Excipial [®] U Hydrolotio	378787	7
	Excipial [®] U Hydrolotio	394125	2
	Excipial [®] U Hydrolotio	401464	2
	Hans Karrer Hydrocream Mi...	LOT22005	1
	Hans Karrer Hydrocream Mi...	LOT23004	1
	Hans Karrer Hydrocream Mi...	LOT24002	3
	Hans Karrer Hydrocream Mi...	LOT24003	1
	Hans Karrer Hydrocream Mi...	LOT24004	5
	Hans Karrer Hydrocream Mi...	LOT24005	2
	Hans Karrer Hydrocream Mi...	LOT25001	1
	Hans Karrer Hydrocream Mi...	LOT25002MAR2028	1
2128114/AHD	Sebexol [®] cream lotion	2128114	1
24042023	Sebexol [®] basic pH 5 formu...	2243126	1
AHD	Sebexol [®] basic pH 5 formu...		1
AHD	Sebexol [®] cream lotion	2040130	1
AHD/ DEVESA	Sebexol [®] cream lotion	2127108	1
Aliance Health Care	Sebexol [®] basic pH 5 formu...	2316117	1
Alliance	Excipial [®] U Hydrolotio	T012	1
Allmiral/Gehe	Amciderm [®] Base cream	418321	1
Almirall / Sanacorp	Amciderm [®] Base cream	48171	2
Almirall Hermal GmbH	Amciderm [®] Base cream	538331	1
Almirall/Alliance	Amciderm [®] Base cream	650341	1
Almirall/Phönix	Amciderm [®] Base cream	12161	1
Almirall/Phönix	Amciderm [®] Base cream	538331	3
Almirall/Phönix	Amciderm [®] Base cream	822351	2
Astellas	Sebexol [®] cream lotion	1504	2
Bombastus	Sebexol [®] basic pH 5 formu...	1346	2
Caelo	Sebexol [®] cream lotion		2
Caelo	Sebexol [®] basic pH 5 formu...	1239	1
Caelo	Sebexol [®] cream lotion	1417	1

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Supplier	Substance	Batch	Spectra
Caelo	Sebexol [®] cream lotion	1430	1
Caelo	Sebexol [®] basic pH 5 formu...	1440	1
Caelo	Sebexol [®] cream lotion	1504	1
Caelo	Sebexol [®] cream lotion	1511	2
Caelo	Sebexol [®] cream lotion	1531	1
Caelo	Sebexol [®] basic pH 5 formu...	1604127	2
Caelo	Sebexol [®] cream lotion	1604129	1
Caelo	Sebexol [®] cream lotion	1605101	3
Caelo	Sebexol [®] basic pH 5 formu...	1620117	2
Caelo	Sebexol [®] cream lotion	1708120	3
Caelo	Sebexol [®] cream lotion	1712223	1
Caelo	Sebexol [®] cream lotion	1719112	1
Caelo	Sebexol [®] cream lotion	1727207	1
Caelo	Sebexol [®] cream lotion	1736105	3
Caelo	Sebexol [®] basic pH 5 formu...	1746116	2
Caelo	Sebexol [®] cream lotion	1802208	1
Caelo	Sebexol [®] cream lotion	1807113	2
Caelo	Sebexol [®] cream lotion	1812123	2
Caelo	Sebexol [®] basic pH 5 formu...	1817126	1
Caelo	Sebexol [®] cream lotion	1817227	1
Caelo	Sebexol [®] cream lotion	1824215	1
Caelo	Sebexol [®] cream lotion	1828110	1
Caelo	Sebexol [®] cream lotion	1836106	1
Caelo	Sebexol [®] basic pH 5 formu...	1851119	2
Caelo	Sebexol [®] cream lotion	19031605	1
Caelo	Sebexol [®] cream lotion	1912119	1
Caelo	Sebexol [®] cream lotion	1912120	1
Caelo	Sebexol [®] cream lotion	4117E-03872	1
Caelo	Excipial [®] U Hydrolotio	L0TR092	1
Chiesi GmbH	Sebexol [®] basic pH 5 formu...	1851119	1
Chiesi	Sebexol [®] cream lotion	218112	1
Devasa/ AHD	Sebexol [®] cream lotion	2124116	1
Deveas/Noweda	Sebexol [®] cream lotion	1901103	1
deversa	Sebexol [®] cream lotion	1935227	5
Deversa	Sebexol [®] basic pH 5 formu...	2031128	2
Deversa/Fiebig	Sebexol [®] cream lotion	1817127	1
Deversa/Fiebig	Sebexol [®] cream lotion	1824115	1
Deversa/Noweda	Sebexol [®] basic pH 5 formu...	1644102	1
Deversa/Noweda	Sebexol [®] basic pH 5 formu...	1712122	1
Deversa/Noweda	Sebexol [®] basic pH 5 formu...	1719111	1
Deversa/Noweda	Sebexol [®] basic pH 5 formu...	1807113	1
Deversa/Noweda	Sebexol [®] basic pH 5 formu...	1817126	1
Deversa/Noweda	Sebexol [®] basic pH 5 formu...	1923107	1
Deversa/Noweda	Sebexol [®] basic pH 5 formu...	2031128	1
Deves/Phönix	Sebexol [®] cream lotion	2127109	1
Devesa Fiebig	Sebexol [®] cream lotion	2128112	1
Devesa / AHD	Sebexol [®] cream lotion	1939227	1
Devesa / AHD	Sebexol [®] cream lotion	1947118	1
Devesa / AHD	Sebexol [®] cream lotion	2009227	2
DEVESA / Anzag	Sebexol [®] cream lotion	1605101	1
DEVESA / Anzag	Sebexol [®] cream lotion	1802208	1
Devesa / Dr. Reingra...	Sebexol [®] basic pH 5 formu...	2009126	1
Devesa / Dr. Reingra...	Sebexol [®] basic pH 5 formu...	2031128	1
Devesa / Dr. Reingra...	Sebexol [®] basic pH 5 formu...	2102114	1
devesa / Fiebig	Sebexol [®] cream lotion	1736106	1
devesa / Fiebig	Sebexol [®] cream lotion	1743125	1

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Supplier	Substance	Batch	Spectra
devesa / Fiebig	Sebexol [®] cream lotion	1746116	1
devesa / Fiebig	Sebexol [®] cream lotion	1802208	1
devesa / Fiebig	Sebexol [®] cream lotion	1812123	1
devesa / Fiebig	Sebexol [®] cream lotion	1828110	1
devesa / Fiebig	Sebexol [®] cream lotion	1912120	1
devesa / Fiebig	Sebexol [®] cream lotion	1935227	1
Devesa / Fiebig	Sebexol [®] cream lotion	2009127	1
Devesa / G	Sebexol [®] basic pH 5 formu. ...	2009126	1
Devesa / Gehe 08.12.18	Sebexol [®] cream lotion	1824215-S20190115Ma7	1
Devesa / Gehe 15.3.18	Sebexol [®] cream lotion	1743225-20180404Ma10	1
Devesa / Gehe	Sebexol [®] cream lotion		1
Devesa / Gehe	Sebexol [®] cream lotion	1517	1
Devesa / Gehe	Sebexol [®] cream lotion	1530	2
Devesa / Gehe	Sebexol [®] cream lotion	1651120	1
Devesa / Gehe	Sebexol [®] cream lotion	1727107	1
Devesa / Gehe	Sebexol [®] cream lotion	1736106	2
Devesa / Gehe	Sebexol [®] cream lotion	1746116	3
Devesa / Gehe	Sebexol [®] basic pH 5 formu. ...	1817126	1
Devesa / Gehe	Sebexol [®] cream lotion	1824215	2
Devesa / Gehe	Sebexol [®] basic pH 5 formu. ...	1851119	1
Devesa / Gehe	Sebexol [®] basic pH 5 formu. ...	1912118	1
Devesa / Gehe	Sebexol [®] cream lotion	1923108	1
Devesa / Gehe	Sebexol [®] basic pH 5 formu. ...	1935126	2
Devesa / Gehe	Sebexol [®] cream lotion	1935127	1
Devesa / Gehe	Sebexol [®] basic pH 5 formu. ...	2009126	3
Devesa / Gehe	Sebexol [®] cream lotion	2009127	1
Devesa / Gehe	Sebexol [®] cream lotion	2019107	2
Devesa / Gehe	Sebexol [®] cream lotion	2045106	1
Devesa / Kehr	Sebexol [®] basic pH 5 formu. ...	1644102	1
Devesa / Noweda	Sebexol [®] cream lotion	1430	1
Devesa / Noweda	Sebexol [®] cream lotion	1531	1
Devesa / Noweda	Sebexol [®] basic pH 5 formu. ...	1620117	1
Devesa / Noweda	Sebexol [®] basic pH 5 formu. ...	1638124	1
Devesa / Noweda	Sebexol [®] cream lotion	1644102	1
Devesa / Noweda	Sebexol [®] basic pH 5 formu. ...	170420S/1620117	1
Devesa / Noweda	Sebexol [®] basic pH 5 formu. ...	170516S/1644102	1
DEVESA / Noweda	Sebexol [®] basic pH 5 formu. ...	1712122	3
Devesa / Noweda	Sebexol [®] cream lotion	1712223	1
Devesa / Noweda	Sebexol [®] cream lotion	1720115	1
Devesa / Noweda	Sebexol [®] cream lotion	1736106	2
Devesa / Noweda	Sebexol [®] cream lotion	1802208	1
Devesa / Noweda	Sebexol [®] cream lotion	1807113	1
Devesa / Noweda	Sebexol [®] cream lotion	1836105	3
Devesa / Noweda	Sebexol [®] cream lotion	1912119	1
Devesa / Noweda	Sebexol [®] cream lotion	2019207	3
Devesa / Noweda	Sebexol [®] cream lotion	2045106	1
Devesa / Phönix	Sebexol [®] cream lotion	1812123	1
Devesa / Phönix	Sebexol [®] cream lotion	2004120	1
Devesa / Phönix	Sebexol [®] cream lotion	2009127	1
Devesa / Sanacorp	Sebexol [®] cream lotion	1828111	2
Devesa /	Sebexol [®] cream lotion	1511	1
Devesa /	Sebexol [®] cream lotion	1812223	1
Devesa /	Sebexol [®] cream lotion	1912119	1
Devesa /	Sebexol [®] cream lotion	1923108	2
DEVESA /G	Sebexol [®] basic pH 5 formu. ...	1912118	1
Devesa /Gehe	Sebexol [®] cream lotion	1901103	1

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Supplier	Substance	Batch	Spectra
DEVESA /K	Sebexol [®] basic pH 5 formu...	1946114	1
Devesa /Noweda	Sebexol [®] cream lotion	1901103	2
Devesa /Phönix	Sebexol [®] cream lotion	1807113	9
Devesa /phönix	Sebexol [®] cream lotion	1947118	1
Devesa Dr. Reingrabe...	Sebexol [®] basic pH 5 formu...	1828110	1
Devesa Dr. Reingrabe...	Sebexol [®] basic pH 5 formu...	1923107	2
Devesa Dr. Reingrabe...	Sebexol [®] cream lotion	2127208	1
Devesa Dr. Reingrabe...	Sebexol [®] cream lotion	2149110	2
Devesa Dr. Reingrabe...	Sebexol [®] basic pH 5 formu...	2124115	1
Devesa Dr. Reingrabe...	Sebexol [®] cream lotion	2124116	1
Devesa Dr. Reingrabe...	Sebexol [®] cream lotion	2127208	3
DEVESA Dr. Reingrabe...	Sebexol [®] cream lotion	2149108	1
DEVESA Dr. Reingrabe...	Sebexol [®] cream lotion	21281147	1
Devesa DR. Reingraber	Sebexol [®] cream lotion	1651121	1
Devesa Dr.Reingraben...	Sebexol [®] cream lotion	1743125	1
Devesa Dr.Reingraben...	Sebexol [®] cream lotion	1817127	3
DEVESA Dr.Reingraber...	Sebexol [®] cream lotion		1
DEVESA Dr.Reingraber...	Sebexol [®] cream lotion	2127108	1
DEVESA Dr.Reingraber...	Sebexol [®] cream lotion	2127109	2
DEVESA Dr.Reingraber...	Sebexol [®] cream lotion	2127208	1
DEVESA Dr.Reingraber...	Sebexol [®] cream lotion	2128112	7
DEVESA Dr.Reingraber...	Sebexol [®] cream lotion	2128114	1
DEVESA Dr.Reingraber...	Sebexol [®] cream lotion	2149108	1
DEVESA Dr.Reingraber...	Sebexol [®] cream lotion	2149110	4
DEVESA Dr.Reingraber GmbH	Sebexol [®] basic pH 5 formu...	1328	1
Devesa Dr.Reingraber GmbH	Sebexol [®] basic pH 5 formu...	1425	1
Devesa Dr.Reingraber GmbH	Sebexol [®] basic pH 5 formu...	1644102	2
Devesa Dr.Reingraber GmbH	Sebexol [®] cream lotion	174611650ml	1
Devesa Dr.Reingraber GmbH	Sebexol [®] cream lotion	1935127	1
Devesa Dr.Reingraber GmbH	Sebexol [®] cream lotion	2009227	1
Devesa Dr.Reingraber GmbH	Sebexol [®] basic pH 5 formu...	2045106	1
Devesa Dr.Reingraber...	Sebexol [®] basic pH 5 formu...	1244	1
Devesa Dr.Reingraber...	Sebexol [®] basic pH 5 formu...	1303	1
Devesa Dr.Reingraber...	Sebexol [®] basic pH 5 formu...	1935126	1
Devesa Dr.Reingraber...	Sebexol [®] basic pH 5 formu...	2031128	1
Devesa Dr.Reingraber...	Sebexol [®] cream lotion	1925121	1
Devesa Dr.Reingraber...	Sebexol [®] cream lotion	1939127	3
Devesa GmbH /Allianc...	Sebexol [®] cream lotion	1712223	1
Devesa GmbH /Allianc...	Sebexol [®] cream lotion	1828110	1
Devesa GmbH /Allianc...	Sebexol [®] cream lotion	1828111	1
Devesa GmbH /Allianc...	Sebexol [®] cream lotion	2128114	1
devesa Noweda	Sebexol [®] cream lotion	1802208	1
devesa phoenix	Sebexol [®] cream lotion	1925121	1
devesa phoenix	Sebexol [®] cream lotion	1947119	1
devesa phoenix	Sebexol [®] cream lotion	2009227	2
Devesa- Phönix	Sebexol [®] basic pH 5 formu...	1604127	1
Devesa-Fa.Gehe	Sebexol [®] cream lotion	1727207/-20180112Ma9	1
Devesa-Fa.Gehe	Sebexol [®] cream lotion	1824215-S20181115Ma2	1
Devesa, Gehe	Sebexol [®] cream lotion	1802208	1
Devesa, Geibo	Sebexol [®] cream lotion	2128114	1
Devesa, Noweda	Sebexol [®] cream lotion	2009227	1
Devesa	Sebexol [®] basic pH 5 formu...		9
Devesa	Sebexol [®] basic pH 5 formu...	1232	1
Devesa	Sebexol [®] basic pH 5 formu...	1239	1
Devesa	Sebexol [®] basic pH 5 formu...	1307	5
DEVESA	Sebexol [®] basic pH 5 formu...	1318	2

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Supplier	Substance	Batch	Spectra
Devesa	Sebexol [®] basic pH 5 formu. ...	1328	5
DEVESA	Sebexol [®] basic pH 5 formu. ...	1328	2
Devesa	Sebexol [®] basic pH 5 formu. ...	1335	2
Devesa	Sebexol [®] basic pH 5 formu. ...	1404	1
Devesa	Sebexol [®] basic pH 5 formu. ...	1407	2
Devesa	Sebexol [®] cream lotion	1417N-03872	1
Devesa	Sebexol [®] basic pH 5 formu. ...	1430	1
Devesa	Sebexol [®] basic pH 5 formu. ...	1440	4
DEVESA	Sebexol [®] basic pH 5 formu. ...	1440	2
DEVESA	Sebexol [®] cream lotion	1505	1
Devesa	Sebexol [®] cream lotion	1510	4
DEVESA	Sebexol [®] cream lotion	1510	1
Devesa	Sebexol [®] basic pH 5 formu. ...	1511	2
DEVESA	Sebexol [®] basic pH 5 formu. ...	1511	1
Devesa	Sebexol [®] basic pH 5 formu. ...	1522	3
Devesa	Sebexol [®] cream lotion	1523	3
DEVESA	Sebexol [®] cream lotion	1523	1
Devesa	Sebexol [®] cream lotion	1524	1
DEVESA	Sebexol [®] cream lotion	1531	1
Devesa	Sebexol [®] basic pH 5 formu. ...	1543	6
Devesa	Sebexol [®] basic pH 5 formu. ...	1604127	4
Devesa	Sebexol [®] cream lotion	1604128	1
Devesa	Sebexol [®] cream lotion	1604129	1
Devesa	Sebexol [®] cream lotion	1604328	1
Devesa	Sebexol [®] cream lotion	1605103	1
Devesa	Sebexol [®] basic pH 5 formu. ...	1620117	2
Devesa	Sebexol [®] basic pH 5 formu. ...	1638124	3
Devesa	Sebexol [®] basic pH 5 formu. ...	1644102	5
DEVESA	Sebexol [®] basic pH 5 formu. ...	1644102	1
DEVESA	Sebexol [®] cream lotion	1651120	2
Devesa	Sebexol [®] cream lotion	1651121	3
Devesa	Sebexol [®] basic pH 5 formu. ...	1683124	1
Devesa	Sebexol [®] cream lotion	1708120	4
DEVESA	Sebexol [®] cream lotion	1708120	1
Devesa	Sebexol [®] basic pH 5 formu. ...	1712122	4
DEVESA	Sebexol [®] basic pH 5 formu. ...	1712122	1
devesa	Sebexol [®] basic pH 5 formu. ...	1719111	3
Devesa	Sebexol [®] basic pH 5 formu. ...	1719111	3
DEVESA	Sebexol [®] basic pH 5 formu. ...	1719111	1
Devesa	Sebexol [®] cream lotion	1727107	2
Devesa	Sebexol [®] cream lotion	1736105	1
DEVESA	Sebexol [®] cream lotion	1736105	1
Devesa	Sebexol [®] cream lotion	1736106	1
Devesa	Sebexol [®] cream lotion	1743125	1
Devesa	Sebexol [®] cream lotion	1743225	1
DEVESA	Sebexol [®] cream lotion	1743225	1
devesa	Sebexol [®] cream lotion	1746116	1
Devesa	Sebexol [®] basic pH 5 formu. ...	1746116	5
Devesa	Sebexol [®] cream lotion	1802108/01	1
DEVESA	Sebexol [®] cream lotion	1802108/01	1
Devesa	Sebexol [®] cream lotion	1802208	1
Devesa	Sebexol [®] basic pH 5 formu. ...	1807113	2
DEVESA	Sebexol [®] basic pH 5 formu. ...	1807113	3
DEVESA	Sebexol [®] cream lotion	1812123	2
Devesa	Sebexol [®] cream lotion	1812223	7
Devesa	Sebexol [®] basic pH 5 formu. ...	1817126	1

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Supplier	Substance	Batch	Spectra
DEVESA	Sebexol [®] basic pH 5 formu...	1817126	1
Devesa	Sebexol [®] cream lotion	1817127	3
Devesa	Sebexol [®] cream lotion	1817227	2
DEVESA	Sebexol [®] cream lotion	1817227	1
Devesa	Sebexol [®] cream lotion	1824115	5
DEVESA	Sebexol [®] cream lotion	1824215	1
Devesa	Sebexol [®] basic pH 5 formu...	1828110	4
Devesa	Sebexol [®] cream lotion	1828111	1
Devesa	Sebexol [®] cream lotion	1836105	1
DEVESA	Sebexol [®] cream lotion	1836106	2
Devesa	Sebexol [®] basic pH 5 formu...	1851119	4
DEVESA	Sebexol [®] basic pH 5 formu...	1851119	1
Devesa	Sebexol [®] cream lotion	1901102	6
Devesa	Sebexol [®] cream lotion	1901103	5
DEVESA	Sebexol [®] cream lotion	1901103	1
Devesa	Sebexol [®] basic pH 5 formu...	1912118	4
DEVESA	Sebexol [®] basic pH 5 formu...	1912118	1
Devesa	Sebexol [®] cream lotion	1912119	3
Devesa	Sebexol [®] cream lotion	1912120	2
DEVESA	Sebexol [®] cream lotion	1912120	1
Devesa	Sebexol [®] basic pH 5 formu...	1923107	6
DEVESA	Sebexol [®] basic pH 5 formu...	1923107	1
Devesa	Sebexol [®] cream lotion	1923108	4
Devesa	Sebexol [®] cream lotion	1923108/06-2022	1
Devesa	Sebexol [®] cream lotion	1925120	1
Devesa	Sebexol [®] cream lotion	1925121	8
DEVESA	Sebexol [®] cream lotion	1925121	1
Devesa	Sebexol [®] basic pH 5 formu...	1935126	2
DEVESA	Sebexol [®] basic pH 5 formu...	1935126	1
Devesa	Sebexol [®] cream lotion	1935127	3
Devesa	Sebexol [®] cream lotion	1935227	5
Devesa	Sebexol [®] cream lotion	1939127	1
Devesa	Sebexol [®] cream lotion	1939227	3
DEVESA	Sebexol [®] cream lotion	1939227	2
Devesa	Sebexol [®] basic pH 5 formu...	1946114	6
Devesa	Sebexol [®] cream lotion	1947118	4
Devesa	Sebexol [®] cream lotion	1947119	5
Devesa	Sebexol [®] cream lotion	2004120	4
Devesa	Sebexol [®] basic pH 5 formu...	2009126	6
DEVESA	Sebexol [®] basic pH 5 formu...	2009126	1
Devesa	Sebexol [®] basic pH 5 formu...	2009126/02	1
Devesa	Sebexol [®] cream lotion	2009127	2
Devesa	Sebexol [®] cream lotion	2009227	4
Devesa	Sebexol [®] cream lotion	201907	1
Devesa	Sebexol [®] cream lotion	2019107	4
Devesa	Sebexol [®] cream lotion	2019207	7
Devesa	Sebexol [®] basic pH 5 formu...	2031128	3
DEVESA	Sebexol [®] basic pH 5 formu...	2031128	1
Devesa	Sebexol [®] cream lotion	2040130	6
DEVESA	Sebexol [®] cream lotion	2040130	1
Devesa	Sebexol [®] cream lotion	2045106	9
Devesa	Sebexol [®] cream lotion	2046109	3
DEVESA	Sebexol [®] cream lotion	2046109	1
devesa	Sebexol [®] basic pH 5 formu...	2102114	1
Devesa	Sebexol [®] basic pH 5 formu...	2102114	1
DEVESA	Sebexol [®] basic pH 5 formu...	2102114	1

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Supplier	Substance	Batch	Spectra
Devesa	Sebexol [®] cream lotion	2103119	6
Devesa	Sebexol [®] cream lotion	2103120	8
devesa	Sebexol [®] basic pH 5 formu. ...	2124115	1
Devesa	Sebexol [®] basic pH 5 formu. ...	2124115	3
DEVESA	Sebexol [®] basic pH 5 formu. ...	2124115	1
Devesa	Sebexol [®] cream lotion	2124116	5
Devesa	Sebexol [®] cream lotion	2124117	7
Devesa	Sebexol [®] cream lotion	212701	1
Devesa	Sebexol [®] cream lotion	2127108	4
Devesa	Sebexol [®] cream lotion	2127109	2
DEVESA	Sebexol [®] cream lotion	2127109	2
Devesa	Sebexol [®] cream lotion	2127208	2
Devesa	Sebexol [®] cream lotion	2128114	1
devesa	Sebexol [®] basic pH 5 formu. ...	2149108	1
Devesa	Sebexol [®] basic pH 5 formu. ...	2149108	3
DEVESA	Sebexol [®] basic pH 5 formu. ...	2149108	2
Devesa	Sebexol [®] basic pH 5 formu. ...	214910812	1
Devesa	Sebexol [®] cream lotion	2149110	1
DEVESA	Sebexol [®] cream lotion	2149110	1
DEVESA	Sebexol [®] cream lotion	2243128	3
DEVESA	Sebexol [®] basic pH 5 formu. ...	2304125	2
Devesa	Sebexol [®] cream lotion	250322/1	1
Devesa	Sebexol [®] cream lotion	9072021	1
Devesa	Sebexol [®] basic pH 5 formu. ...	I232	1
Devesa	Sebexol [®] basic pH 5 formu. ...	I307	1
Devesa/ Noweda	Sebexol [®] basic pH 5 formu. ...	1712122	1
Devesa/ Noweda	Sebexol [®] cream lotion	1817227	1
Devesa/ AHD	Sebexol [®] cream lotion	2019107	1
Devesa/ AHD	Sebexol [®] cream lotion	2127108	3
Devesa/ Ebert	Sebexol [®] basic pH 5 formu. ...	1817126	1
Devesa/ Fiebig	Sebexol [®] basic pH 5 formu. ...	1338	1
Devesa/ Fiebig	Sebexol [®] cream lotion	1447	1
Devesa/ Fiebig	Sebexol [®] cream lotion	1712223	2
Devesa/ Fiebig	Sebexol [®] cream lotion	1935227	1
Devesa/ Noweda	Sebexol [®] cream lotion	1736105	1
Devesa/ Noweda	Sebexol [®] cream lotion	1802208	1
Devesa/ Noweda	Sebexol [®] cream lotion	1807113	1
Devesa/ Noweda	Sebexol [®] cream lotion	1901103	1
Devesa/ Noweda	Sebexol [®] cream lotion	1935227	2
Devesa/ Noweda	Sebexol [®] cream lotion	1939227	4
Devesa/ Noweda	Sebexol [®] cream lotion	1947118	1
Devesa/ Noweda	Sebexol [®] cream lotion	1947119	2
DEVESA/ Noweda	Sebexol [®] basic pH 5 formu. ...	2124115	1
Devesa/ Noweda	Sebexol [®] cream lotion	2124116	1
Devesa/ Phoenix	Sebexol [®] basic pH 5 formu. ...	1543	1
Devesa/ Phoenix	Sebexol [®] cream lotion	1620117	1
Devesa/ Phoenix	Sebexol [®] cream lotion	1817127	1
DEVESA/ Phoenix	Sebexol [®] cream lotion	1939127/09	1
Devesa/ Phoenix	Sebexol [®] basic pH 5 formu. ...	2127106	5
Devesa/ Phönix	Sebexol [®] cream lotion	1524	1
Devesa/ Phönix	Sebexol [®] cream lotion	1727207	1
Devesa/ Phönix	Sebexol [®] cream lotion	1736105	2
Devesa/ Phönix	Sebexol [®] cream lotion	1736106	6
Devesa/ Phönix	Sebexol [®] cream lotion	1743225	2
Devesa/ Phönix	Sebexol [®] cream lotion	1812223	3
Devesa/ Phönix	Sebexol [®] cream lotion	1824215	1

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Supplier	Substance	Batch	Spectra
Devesa/ Phönix	Sebexol [®] cream lotion	1901103	1
DEVESA/ Phönix	Sebexol [®] cream lotion	2040130	1
Devesa/ Sanacorp	Sebexol [®] cream lotion	1912120	1
Devesa/ Sanacorp	Sebexol [®] cream lotion	1923108	1
Devesa/ Sanacorp	Sebexol [®] cream lotion	1925121	1
Devesa/ Sanacorp	Sebexol [®] cream lotion	1939127	1
Devesa/ Sanacorp	Sebexol [®] cream lotion	20042120	1
Devesa/	Sebexol [®] cream lotion		2
Devesa/	Sebexol [®] cream lotion	1504	2
Devesa/	Sebexol [®] cream lotion	1524	1
Devesa/	Sebexol [®] cream lotion	1604129	4
Devesa/	Sebexol [®] cream lotion	1644102	1
Devesa/	Sebexol [®] cream lotion	17433225	1
Devesa/	Sebexol [®] cream lotion	1947118	1
Devesa/AHD	Sebexol [®] basic pH 5 formu...	1131	2
Devesa/AHD	Sebexol [®] basic pH 5 formu...	1245	4
Devesa/AHD	Sebexol [®] basic pH 5 formu...	1328	7
Devesa/AHD	Sebexol [®] cream lotion	1912119	1
Devesa/AHD	Sebexol [®] cream lotion	1947118	1
Devesa/AHD	Sebexol [®] cream lotion	2009127	2
Devesa/AHD	Sebexol [®] cream lotion	2040130	1
Devesa/AHD	Sebexol [®] cream lotion	2045106	1
Devesa/AHD	Sebexol [®] cream lotion	2103119	1
Devesa/AHD	Sebexol [®] cream lotion	2103120	1
Devesa/AHD	Sebexol [®] cream lotion	2128112	1
Devesa/AHD	Sebexol [®] cream lotion	2128114	1
Devesa/Alliance	Sebexol [®] basic pH 5 formu...	1644102	1
Devesa/Alliance	Sebexol [®] cream lotion	1923108	2
Devesa/Alliance	Sebexol [®] cream lotion	1935127	2
Devesa/Alliance	Sebexol [®] cream lotion	1939227	1
Devesa/Alliance	Sebexol [®] basic pH 5 formu...	1946114	2
Devesa/Alliance	Sebexol [®] basic pH 5 formu...	2009126	5
Devesa/Alliance	Sebexol [®] cream lotion	2019207	1
Devesa/Alliance	Sebexol [®] basic pH 5 formu...	2031128	16
Devesa/Alliance	Sebexol [®] cream lotion	2046109	2
Devesa/Alliance	Sebexol [®] basic pH 5 formu...	2149108	6
Devesa/Alliance	Sebexol [®] basic pH 5 formu...	2243126	1
Devesa/alliance	Sebexol [®] basic pH 5 formu...	2316117	11
Devesa/alliance	Sebexol [®] basic pH 5 formu...	2316117/04	1
Devesa/Anzag	Sebexol [®] cream lotion		3
Devesa/Anzag	Sebexol [®] cream lotion	1836105	1
Devesa/Anzag	Sebexol [®] cream lotion	1912119	1
Devesa/Anzag	Sebexol [®] cream lotion	1939227	1
Devesa/Anzag	Sebexol [®] cream lotion	2004120	1
Devesa/Anzag	Sebexol [®] cream lotion	2045106	1
Devesa/Anzag	Sebexol [®] cream lotion	2103120	1
Devesa/Anzag	Sebexol [®] cream lotion	2124117	1
DEVESA/Anzag	Sebexol [®] cream lotion	2127208	1
Devesa/fiebig	Sebexol [®] cream lotion		1
Devesa/Fiebig	Sebexol [®] cream lotion		1
Devesa/Fiebig	Sebexol [®] cream lotion	1426	1
Devesa/Fiebig	Sebexol [®] cream lotion	1511	1
Devesa/Fiebig	Sebexol [®] cream lotion	1712123	2
Devesa/Fiebig	Sebexol [®] cream lotion	1736105	5
Devesa/Fiebig	Sebexol [®] cream lotion	1824115	2
DEVESA/Fiebig	Sebexol [®] cream lotion	1925121	1

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Supplier	Substance	Batch	Spectra
Devesa/Fiebig	Sebexol [®] cream lotion	1935127	2
DEVESA/Fiebig	Sebexol [®] cream lotion	1935127	1
DEVESA/Fiebig	Sebexol [®] cream lotion	1939227	1
Devesa/Fiebig	Sebexol [®] cream lotion	1947118	6
DEVESA/Fiebig	Sebexol [®] cream lotion	1947118	1
Devesa/Fiebig	Sebexol [®] cream lotion	1947119	2
DEVESA/Fiebig	Sebexol [®] cream lotion	1947119	1
Devesa/Fiebig	Sebexol [®] cream lotion	2004120	1
Devesa/Fiebig	Sebexol [®] cream lotion	2009127	4
Devesa/Fiebig	Sebexol [®] cream lotion	201107	2
Devesa/Fiebig	Sebexol [®] cream lotion	2019107	6
Devesa/Fiebig	Sebexol [®] cream lotion	2019207	1
Devesa/Fiebig	Sebexol [®] cream lotion	2040130	2
Devesa/Fiebig	Sebexol [®] cream lotion	2045106	3
Devesa/Fiebig	Sebexol [®] cream lotion	2046109	1
Devesa/Fiebig	Sebexol [®] cream lotion	2103119	4
Devesa/Fiebig	Sebexol [®] cream lotion	2103120	2
Devesa/Fiebig	Sebexol [®] cream lotion	2124116	4
Devesa/Fiebig	Sebexol [®] cream lotion	2124117	2
Devesa/Fiebig	Sebexol [®] cream lotion	2127109	1
Devesa/Fiebig	Sebexol [®] cream lotion	2128112	2
Devesa/Fiebig	Sebexol [®] cream lotion	2128114	2
Devesa/Fiebig	Sebexol [®] cream lotion	2149108	1
Devesa/Fiebig	Sebexol [®] cream lotion	2149110	1
Devesa/Fiebig	Sebexol [®] cream lotion	218112	1
Devesa/Gehe	Sebexol [®] basic pH 5 formu. ...		2
devesa/gehe	Sebexol [®] basic pH 5 formu. ...	1346	1
devesa/gehe	Sebexol [®] basic pH 5 formu. ...	1356	1
Devesa/Gehe	Sebexol [®] cream lotion	1504	1
Devesa/Gehe	Sebexol [®] cream lotion	1644102	1
Devesa/Gehe	Sebexol [®] cream lotion	1651121	1
Devesa/Gehe	Sebexol [®] cream lotion	1712123	1
Devesa/Gehe	Sebexol [®] cream lotion	1817227	1
Devesa/Gehe	Sebexol [®] cream lotion	1828111	1
Devesa/Gehe	Sebexol [®] cream lotion	1836106	1
Devesa/Gehe	Sebexol [®] basic pH 5 formu. ...	1851119	1
Devesa/Gehe	Sebexol [®] basic pH 5 formu. ...	1912118	1
Devesa/Gehe	Sebexol [®] cream lotion	1912119	1
Devesa/Gehe	Sebexol [®] basic pH 5 formu. ...	1923107	2
Devesa/Gehe	Sebexol [®] basic pH 5 formu. ...	1935126	2
Devesa/Gehe	Sebexol [®] cream lotion	1939127	1
Devesa/Gehe	Sebexol [®] basic pH 5 formu. ...	1946114	1
Devesa/Gehe	Sebexol [®] cream lotion	2009127	1
Devesa/Gehe	Sebexol [®] cream lotion	2009227	2
Devesa/Gehe	Sebexol [®] cream lotion	2124116	1
Devesa/Gehe	Sebexol [®] cream lotion	2127108	2
Devesa/Gehe	Sebexol [®] cream lotion	2127208	1
DEVESA/Gehe	Sebexol [®] cream lotion	2127208	1
Devesa/Gehe	Sebexol [®] cream lotion	2128114	5
Devesa/Gehe	Sebexol [®] cream lotion	2149110	4
Devesa/Gehe	Sebexol [®] cream lotion	2243128	5
Devesa/gehe	Sebexol [®] basic pH 5 formu. ...	2304125	1
Devesa/Jenne	Sebexol [®] cream lotion	2103119	2
Devesa/Kehr	Sebexol [®] basic pH 5 formu. ...	1407	2
Devesa/Kehr	Sebexol [®] basic pH 5 formu. ...	1620117	1
Devesa/Kehr	Sebexol [®] basic pH 5 formu. ...	1923107	1

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Supplier	Substance	Batch	Spectra
Devesa/Kehr	Sebexol [®] basic pH 5 formu...	1946114	1
Devesa/Kehr	Sebexol [®] basic pH 5 formu...	1946114/11	1
Devesa/Kehr	Sebexol [®] basic pH 5 formu...	2009126	3
Devesa/Kehr	Sebexol [®] basic pH 5 formu...	2102114	2
Devesa/Kehr	Sebexol [®] basic pH 5 formu...	2124115	1
Devesa/Kehr/25.05.2020	Sebexol [®] cream lotion	2004120	2
Devesa/Krieger	Sebexol [®] cream lotion	1802108	1
Devesa/Krieger	Sebexol [®] cream lotion	1901102	1
Devesa/Krieger	Sebexol [®] cream lotion	1901103	1
Devesa/Krieger	Sebexol [®] cream lotion	1939227	1
Devesa/Krieger	Sebexol [®] cream lotion	1947118	1
Devesa/Krieger	Sebexol [®] cream lotion	2004120	2
Devesa/Noweda	Sebexol [®] cream lotion	2124166	1
Devesa/NOW	Sebexol [®] cream lotion		1
Devesa/NOW	Sebexol [®] cream lotion	1504	2
Devesa/NOW	Sebexol [®] cream lotion	1504/01	1
Devesa/NOW	Sebexol [®] cream lotion	1523	1
Devesa/NOW	Sebexol [®] cream lotion	1552	1
Devesa/NOW	Sebexol [®] cream lotion	1604129	1
Devesa/NOW	Sebexol [®] cream lotion	1604228	1
Devesa/NOW	Sebexol [®] cream lotion	1644102	1
Devesa/NOW	Sebexol [®] cream lotion	1901103	1
Devesa/NOW	Sebexol [®] cream lotion	2019207	1
Devesa/Noweda	Sebexol [®] cream lotion		3
Devesa/Noweda	Sebexol [®] basic pH 5 formu...	1430	1
Devesa/Noweda	Sebexol [®] basic pH 5 formu...	1440	2
Devesa/Noweda	Sebexol [®] cream lotion	1447	3
Devesa/Noweda	Sebexol [®] cream lotion	1543	1
DEVESA/Noweda	Sebexol [®] basic pH 5 formu...	1543	1
Devesa/Noweda	Sebexol [®] basic pH 5 formu...	1604127	1
DEVESA/Noweda	Sebexol [®] basic pH 5 formu...	1604127	1
Devesa/Noweda	Sebexol [®] cream lotion	1604228	6
Devesa/Noweda	Sebexol [®] cream lotion	1604328	5
Devesa/Noweda	Sebexol [®] cream lotion	1605103	1
Devesa/Noweda	Sebexol [®] cream lotion	1605201	3
DEVESA/Noweda	Sebexol [®] cream lotion	1605201	2
Devesa/Noweda	Sebexol [®] basic pH 5 formu...	1638124	2
Devesa/Noweda	Sebexol [®] cream lotion	1651120	1
Devesa/Noweda	Sebexol [®] cream lotion	1651121	1
Devesa/Noweda	Sebexol [®] cream lotion	1708120	1
Devesa/Noweda	Sebexol [®] cream lotion	1712123	1
Devesa/Noweda	Sebexol [®] basic pH 5 formu...	1719111/05	1
Devesa/Noweda	Sebexol [®] cream lotion	1719112	1
Devesa/Noweda	Sebexol [®] cream lotion	1720115	1
Devesa/Noweda	Sebexol [®] cream lotion	1736105	1
Devesa/Noweda	Sebexol [®] cream lotion	1736106	1
Devesa/Noweda	Sebexol [®] cream lotion	1743225	1
Devesa/Noweda	Sebexol [®] basic pH 5 formu...	1807113	2
Devesa/Noweda	Sebexol [®] cream lotion	1812223	1
Devesa/Noweda	Sebexol [®] basic pH 5 formu...	1817126	1
Devesa/Noweda	Sebexol [®] cream lotion	1817227	3
Devesa/Noweda	Sebexol [®] cream lotion	1824115	1
Devesa/Noweda	Sebexol [®] basic pH 5 formu...	1828110	2
Devesa/Noweda	Sebexol [®] basic pH 5 formu...	1828110/07	1
Devesa/Noweda	Sebexol [®] cream lotion	1828111	2
Devesa/Noweda	Sebexol [®] cream lotion	1901102	1

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Supplier	Substance	Batch	Spectra
Devesa/Noweda	Sebexol [®] cream lotion	1912119	1
Devesa/Noweda	Sebexol [®] cream lotion	1923108	1
Devesa/Noweda	Sebexol [®] cream lotion	1935127	2
Devesa/Noweda	Sebexol [®] cream lotion	1935227	1
Devesa/Noweda	Sebexol [®] cream lotion	1939127	2
Devesa/Noweda	Sebexol [®] cream lotion	1939227	4
Devesa/Noweda	Sebexol [®] basic pH 5 formu. . .	1946114	3
Devesa/Noweda	Sebexol [®] cream lotion	1947118	2
Devesa/Noweda	Sebexol [®] cream lotion	1947119	10
Devesa/Noweda	Sebexol [®] cream lotion	1947119/11	1
Devesa/Noweda	Sebexol [®] cream lotion	2004120	4
Devesa/Noweda	Sebexol [®] cream lotion	200412D	1
Devesa/Noweda	Sebexol [®] basic pH 5 formu. . .	2009126	1
Devesa/Noweda	Sebexol [®] cream lotion	2009227	3
Devesa/Noweda	Sebexol [®] cream lotion	2040130	4
Devesa/Noweda	Sebexol [®] cream lotion	2045106	1
Devesa/Noweda	Sebexol [®] cream lotion	2103119	1
DEVESA/Noweda	Sebexol [®] cream lotion	2124116	1
Devesa/Noweda	Sebexol [®] cream lotion	2127108	4
DEVESA/Noweda	Sebexol [®] cream lotion	2127108	5
Devesa/Noweda	Sebexol [®] cream lotion	2127208	2
Devesa/Noweda	Sebexol [®] cream lotion	2128112	3
Devesa/Noweda	Sebexol [®] cream lotion	2128114	1
Devesa/Noweda	Sebexol [®] cream lotion	2149110	2
Devesa/Noweda	Sebexol [®] cream lotion	2304125	1
Devesa/Noweda	Sebexol [®] cream lotion	2304126	1
DEVESA/Phoenix	Sebexol [®] basic pH 5 formu. . .	1446/11	1
Devesa/Phoenix	Sebexol [®] cream lotion	1511	1
Devesa/Phoenix	Sebexol [®] cream lotion	1746116	1
Devesa/Phoenix	Sebexol [®] cream lotion	1807113	3
Devesa/Phoenix	Sebexol [®] cream lotion	1824215	1
Devesa/Phoenix	Sebexol [®] cream lotion	1828111	2
Devesa/Phoenix	Sebexol [®] cream lotion	1901102	2
Devesa/Phoenix	Sebexol [®] cream lotion	1901103	1
Devesa/Phoenix	Sebexol [®] cream lotion	1912120	3
Devesa/Phoenix	Sebexol [®] cream lotion	1925121	1
DEVESA/PHOENIX	Sebexol [®] cream lotion	1935127	1
Devesa/Phoenix	Sebexol [®] cream lotion	1939127	1
Devesa/Phoenix	Sebexol [®] cream lotion	1947118	1
DEVESA/PHOENIX	Sebexol [®] cream lotion	1947118	2
Devesa/Phoenix	Sebexol [®] cream lotion	1947119	1
Devesa/Phoenix	Sebexol [®] cream lotion	2004120	2
Devesa/Phoenix	Sebexol [®] cream lotion	2009227	3
DEVESA/PHOENIX	Sebexol [®] cream lotion	2009227	1
Devesa/Phoenix	Sebexol [®] cream lotion	2019107	1
DEVESA/PHOENIX	Sebexol [®] cream lotion	2019107	1
Devesa/Phoenix	Sebexol [®] cream lotion	2045106	1
DEVESA/PHOENIX	Sebexol [®] cream lotion	2046109	1
Devesa/Phoenix	Sebexol [®] basic pH 5 formu. . .	2102114	17
Devesa/Phoenix	Sebexol [®] basic pH 5 formu. . .	2124115	12
Devesa/Phoenix	Sebexol [®] cream lotion	2124117	2
DEVESA/PHOENIX	Sebexol [®] cream lotion	2127208	2
Devesa/Phoenix	Sebexol [®] basic pH 5 formu. . .	2304125	1
Devesa/Phömix	Sebexol [®] cream lotion	1712223	2
Devesa/Phömix	Sebexol [®] basic pH 5 formu. . .	1543	3
Devesa/Phömix	Sebexol [®] basic pH 5 formu. . .	1620117	2

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Supplier	Substance	Batch	Spectra
Devesa/Phönix	Sebexol [®] basic pH 5 formu...	1638124	2
Devesa/Phönix	Sebexol [®] cream lotion	1708120	1
Devesa/Phönix	Sebexol [®] basic pH 5 formu...	1712122	2
DEVESA/Phönix	Sebexol [®] basic pH 5 formu...	1719111	1
devesa/Phönix	Sebexol [®] cream lotion	1727107	1
Devesa/Phönix	Sebexol [®] cream lotion	1727207	1
devesa/Phönix	Sebexol [®] cream lotion	1743125	5
devesa/Phönix	Sebexol [®] cream lotion	1746116	8
Devesa/Phönix	Sebexol [®] cream lotion	1746116	1
devesa/Phönix	Sebexol [®] cream lotion	1802208	5
Devesa/Phönix	Sebexol [®] cream lotion	1807113	2
DEVESA/Phönix	Sebexol [®] basic pH 5 formu...	1807113	1
Devesa/Phönix	Sebexol [®] cream lotion	1807113/02	1
Devesa/Phönix	Sebexol [®] cream lotion	1817227	1
devesa/Phönix	Sebexol [®] cream lotion	18201402	1
Devesa/Phönix	Sebexol [®] cream lotion	1824115	2
devesa/Phönix	Sebexol [®] cream lotion	1824215	2
Devesa/Phönix	Sebexol [®] cream lotion	1824215	1
DEVESA/Phönix	Sebexol [®] basic pH 5 formu...	1828110	1
Devesa/Phönix	Sebexol [®] cream lotion	1828111	19
Devesa/Phönix	Sebexol [®] cream lotion	1836105	2
DEVESA/Phönix	Sebexol [®] basic pH 5 formu...	1851119	1
DEVESA/Phönix	Sebexol [®] cream lotion	1851119	1
Devesa/Phönix	Sebexol [®] cream lotion	1901102	2
Devesa/Phönix	Sebexol [®] cream lotion	1901103	6
Devesa/Phönix	Sebexol [®] cream lotion	19107	1
Devesa/Phönix	Sebexol [®] cream lotion	1912119	1
Devesa/Phönix	Sebexol [®] cream lotion	1912120	3
Devesa/Phönix	Sebexol [®] cream lotion	1923108	9
Devesa/Phönix	Sebexol [®] cream lotion	1925121	1
Devesa/Phönix	Sebexol [®] cream lotion	1935127	1
Devesa/Phönix	Sebexol [®] cream lotion	1935227	6
Devesa/Phönix	Sebexol [®] cream lotion	1939127	7
DEVESA/Phönix	Sebexol [®] cream lotion	1947119	2
Devesa/Phönix	Sebexol [®] cream lotion	2004120	2
Devesa/Phönix	Sebexol [®] cream lotion	2009227	8
Devesa/Phönix	Sebexol [®] cream lotion	2019107	1
Devesa/Phönix	Sebexol [®] basic pH 5 formu...	2031128	2
Devesa/Phönix	Sebexol [®] cream lotion	2045106	1
Devesa/Phönix	Sebexol [®] cream lotion	2124116	2
DEVESA/Phönix	Sebexol [®] cream lotion	2124117	1
Devesa/Phönix	Sebexol [®] cream lotion	2127108	1
Devesa/Phönix	Sebexol [®] cream lotion	2127208	1
DEVESA/Phönix	Sebexol [®] cream lotion	2127208	1
Devesa/Phönix	Sebexol [®] cream lotion	2128114	1
Devesa/Sanacorp WE: ...	Sebexol [®] cream lotion	1651121	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu...	1440	1
Devesa/Sanacorp	Sebexol [®] cream lotion	1511	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu...	1522	1
Devesa/Sanacorp	Sebexol [®] cream lotion	1530	2
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu...	1543	4
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu...	1620117	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu...	1638124	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu...	1644102	2
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu...	1712122	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu...	1719111	1

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Supplier	Substance	Batch	Spectra
Devesa/Sanacorp	Sebexol [®] cream lotion	1743125	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	1746116	2
Devesa/Sanacorp	Sebexol [®] cream lotion	1802108	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	1807113	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	1817126	1
Devesa/Sanacorp	Sebexol [®] cream lotion	1817127	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	1828110	3
Devesa/Sanacorp	Sebexol [®] cream lotion	1828111	4
Devesa/Sanacorp	Sebexol [®] cream lotion	1836105	1
Devesa/Sanacorp	Sebexol [®] cream lotion	1836106	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	1851119	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	187126/06	1
Devesa/Sanacorp	Sebexol [®] cream lotion	1901102	2
Devesa/Sanacorp	Sebexol [®] cream lotion	1912120	2
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	1923107	1
Devesa/Sanacorp	Sebexol [®] cream lotion	1925121	2
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	1935126	4
Devesa/Sanacorp	Sebexol [®] cream lotion	1935127	1
Devesa/Sanacorp	Sebexol [®] cream lotion	1935227	1
Devesa/Sanacorp	Sebexol [®] cream lotion	1939227	1
Devesa/Sanacorp	Sebexol [®] cream lotion	1947118	2
Devesa/Sanacorp	Sebexol [®] cream lotion	1947119	1
DEVEsa/Sanacorp	Sebexol [®] cream lotion	2004120	2
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	2009126	2
Devesa/Sanacorp	Sebexol [®] cream lotion	2019207	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	2031128	5
Devesa/Sanacorp	Sebexol [®] cream lotion	2040130	3
Devesa/Sanacorp	Sebexol [®] cream lotion	2103119	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	2124115	7
Devesa/Sanacorp	Sebexol [®] cream lotion	2124117	1
Devesa/Sanacorp	Sebexol [®] cream lotion	2127108	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formu. ...	2243126	1
Devesa/Sanacorp	Sebexol [®] cream lotion	2304125	1
DevesaSanacorp	Sebexol [®] cream lotion	1912119	1
Devesea	Sebexol [®] cream lotion	1604128	1
Dewesa/Kehr	Sebexol [®] basic pH 5 formu. ...	1817126	1
Dewesa/Kehr	Sebexol [®] basic pH 5 formu. ...	1923107	1
Divesa	Sebexol [®] cream lotion	1812223	1
Dr Reinhard GmbH- Kehr	Sebexol [®] basic pH 5 formu. ...	1620117	1
Dr. Reingraber GmbH ...	Sebexol [®] cream lotion	1824115	1
Dr. Reingraber GmbH	Sebexol [®] cream lotion	1605103	1
Dr. Reingraber GmbH	Sebexol [®] basic pH 5 formu. ...	1708120	1
Dr. Reingraber GmbH	Sebexol [®] cream lotion	1817227	1
Dr. Reingraber GmbH	Sebexol [®] cream lotion	1923108	1
Dr. Reingraber GmbH	Sebexol [®] cream lotion	1939127	1
Dr. Reingraber GmbH	Sebexol [®] cream lotion	2103119	2
Dr. Reingraber GmbH	Sebexol [®] cream lotion	2127108	1
Dr. Reingraber GmbH/...	Sebexol [®] basic pH 5 formu. ...	2031128	1
Dr. Reingraber GmbH/...	Sebexol [®] cream lotion	2103119	2
Dr. Wolff	Sebexol [®] cream lotion		1
Dr.Reingraber GmbH	Sebexol [®] basic pH 5 formu. ...	1232	1
Dr.Reingraber/sanacorp	Sebexol [®] basic pH 5 formu. ...	1719111	1
Dr.Reingraber/sanacorp	Sebexol [®] basic pH 5 formu. ...	1923107	1
Eigenherstellung	Sebexol [®] basic pH 5 formu. ...	1328	1
Euro OTC	Sebexol [®] cream lotion	1727207	1
Fa. Devesa/Gehe	Sebexol [®] cream lotion	2009227	1

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Supplier	Substance	Batch	Spectra
Fa. Devesa/Noweda	Sebexol [®] cream lotion	1912120	1
Fa. Devesa/Noweda	Sebexol [®] cream lotion	1935227	2
Fa. Devesa/Noweda	Sebexol [®] cream lotion	1947118	1
Fa. Devesa/Noweda	Sebexol [®] cream lotion	1947119	1
Fa. Devesa/Noweda	Sebexol [®] cream lotion	2004120	5
Fa. Devesa/Noweda	Sebexol [®] cream lotion	2009127	1
Fa. Devesa/Noweda	Sebexol [®] cream lotion	2040130	1
Fa. Devesa/Noweda	Sebexol [®] cream lotion	2045106	1
Fa. Devesa/Noweda	Sebexol [®] cream lotion	2046109	2
Fa. Devesa/Noweda	Sebexol [®] cream lotion	2103120	3
Fa. Devesa/Noweda	Sebexol [®] cream lotion	2127208	3
Fa. Devesa/Gehe	Sebexol [®] cream lotion	2019107	1
Fa. Devesa/Noweda	Sebexol [®] cream lotion	2124117	1
Fagron	Sebexol [®] basic pH 5 formu...	1425	1
Fagron	Nourivan [™] Antiox	150325	1
Fagron	Nourivan [™] Antiox	1503258	3
Fagron	Sebexol [®] basic pH 5 formu...	1510	2
Fagron	Sebexol [®] cream lotion	1517	1
Fagron	Amciderm [®] Base cream	23102017	1
Fiebig / Devesa	Sebexol [®] cream lotion	2019107	1
FIEBIG; HERSTELLER D...	Sebexol [®] cream lotion	2004120	1
Fiebig	Sebexol [®] basic pH 5 formu...	1511	2
Fiebig	Sebexol [®] cream lotion	1605101	2
Fiebig	Sebexol [®] cream lotion	1802108	1
Fiebig	Sebexol [®] cream lotion	1812223	1
Fiebig	Sebexol [®] cream lotion	1828111	1
Fiebig	Sebexol [®] cream lotion	1912119	1
Fiebig	Sebexol [®] cream lotion	1912120	1
Fiebig/Devesa	Sebexol [®] cream lotion	1817227	1
Fiebig/Devesa	Sebexol [®] cream lotion	1836105	2
Fiebig/Devesa	Sebexol [®] cream lotion	1912120	1
Fiebig/Devesa	Sebexol [®] cream lotion	2009127	1
Galderma / Alliance ...	Excipial [®] U Hydrolotio	340781	2
Galderma Internation...	Excipial [®] U Hydrolotio	346815	1
Galderma Internation...	Excipial [®] U Hydrolotio	V042	1
Galderma Laboratoriu...	Excipial [®] U Hydrolotio	318208	1
Galderma Laboratoriu...	Excipial [®] U Hydrolotio	340781	1
Galderma Laboratoriu...	Excipial [®] U Hydrolotio	344143	2
Galderma Laboratoriu...	Excipial [®] U Hydrolotio	344145	1
Galderma Laboratoriu...	Excipial [®] U Hydrolotio	357789	1
Galderma Laboratoriu...	Excipial [®] U Hydrolotio	365111	1
Galderma	Excipial [®] U Hydrolotio	1107483	1
Galderma	Excipial [®] U Hydrolotio	172481	1
Galderma	Excipial [®] U Hydrolotio	302972	2
Galderma	Excipial [®] U Hydrolotio	306123	1
Galderma	Excipial [®] U Hydrolotio	315815	1
Galderma	Excipial [®] U Hydrolotio	318203	1
Galderma	Excipial [®] U Hydrolotio	344143	1
Galderma	Excipial [®] U Hydrolotio	346815	1
Galderma	Excipial [®] U Hydrolotio	50857	1
Galderma	Excipial [®] U Hydrolotio	L0TR054	1
Galderma	Excipial [®] U Hydrolotio	T011	1
Galderma	Excipial [®] U Hydrolotio	V042	1
Galderma/ Fiebig	Excipial [®] U Hydrolotio	L0TV022	1
Galderma/ Gehe	Excipial [®] U Hydrolotio	L0TR053	1
Galderma/ Phoenix	Excipial [®] U Hydrolotio	324614	1

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Supplier	Substance	Batch	Spectra
Galderma/ Phoenix	Excipial [®] U Hydrolotio	331554	4
Galderma/ Phoenix	Excipial [®] U Hydrolotio	344143	2
Galderma/ Phoenix	Excipial [®] U Hydrolotio	344145	1
Galderma/ Phoenix/ 0...	Excipial [®] U Hydrolotio	302972	1
Galderma/ Phoenix/ 0...	Excipial [®] U Hydrolotio	327533	1
Galderma/ Phönix	Excipial [®] U Hydrolotio	340781	1
Galderma/AEP	Excipial [®] U Hydrolotio	324226	2
Galderma/Alliance	Excipial [®] U Hydrolotio	365111	4
Galderma/Alliance	Excipial [®] U Hydrolotio	50723	1
Galderma/Alliance	Excipial [®] U Hydrolotio	T072	2
Galderma/Anzag	Excipial [®] U Hydrolotio	1(172141)	1
Galderma/Anzag	Excipial [®] U Hydrolotio	2(302972)	1
Galderma/Anzag	Excipial [®] U Hydrolotio	3(302972)	1
Galderma/Anzag	Excipial [®] U Hydrolotio	4(302972)	1
Galderma/Anzag	Excipial [®] U Hydrolotio	5(302972)	1
Galderma/Anzag	Excipial [®] U Hydrolotio	6(317160)	1
Galderma/Gehe	Excipial [®] U Hydrolotio	164957	2
Galderma/Gehe	Excipial [®] U Hydrolotio	50723	1
Galderma/Gehe	Excipial [®] U Hydrolotio	S014	1
Galderma/Gehe	Excipial [®] U Hydrolotio	V052	1
Galderma/Noweda	Excipial [®] U Hydrolotio	164957	1
Galderma/Noweda	Excipial [®] U Hydrolotio	340006	1
Galderma/Noweda	Excipial [®] U Hydrolotio	344143	1
Galderma/Noweda	Excipial [®] U Hydrolotio	357789	1
Galderma/Noweda	Excipial [®] U Hydrolotio	R054	1
Galderma/P	Excipial [®] U Hydrolotio	V051	1
Galderma/Phoenix	Excipial [®] U Hydrolotio	378787	1
galderma/phönix	Excipial [®] U Hydrolotio	327533	1
galderma/phönix	Excipial [®] U Hydrolotio	332020	1
Galderma/Phönix	Excipial [®] U Hydrolotio	T013	1
Galderma/Phönix	Excipial [®] U Hydrolotio	V011	1
galderma/sanacorp	Excipial [®] U Hydrolotio	331554	1
Galderna/Sanacorp	Excipial [®] U Hydrolotio	340781	1
GEHE / DEVESA	Sebexol [®] cream lotion	2009127	1
Gehe	Sebexol [®] cream lotion	1605103	1
Gehe	Sebexol [®] cream lotion	1727107	1
Gehe	Sebexol [®] basic pH 5 formu. ...	1935126	2
Gehe	Sebexol [®] cream lotion	2009227	1
Gehe	Sebexol [®] cream lotion	2304125	4
Gehe	Sebexol [®] cream lotion	2304126	4
GEHE	Sebexol [®] cream lotion	2316118	6
Gehe	Sebexol [®] cream lotion	2316119	4
Gehe	Sebexol [®] cream lotion	2337114	1
Gehe	Sebexol [®] cream lotion	2414102	4
Gehe	Sebexol [®] cream lotion	2436106	5
Gehe	Sebexol [®] cream lotion	2513124	4
Gehe/Devesa	Sebexol [®] cream lotion		1
Geibo/Devesa	Sebexol [®] cream lotion	1947118	1
Hans Karrer / Anzag	Hans Karrer Hydrocream Mi. ...	18002	1
Hans Karrer / Noweda	Hans Karrer Hydrocream Mi. ...	20007	1
Hans Karrer / Phönix	Hans Karrer Hydrocream Mi. ...	19003	2
Hans Karrer / Phönix	Hans Karrer Hydrocream Mi. ...	L0T20001	1
Hans Karrer GmbH / A...	Hans Karrer Hydrocream Mi. ...	18004	2
Hans Karrer GmbH / P...	Hans Karrer Hydrocream Mi. ...	L0T21001	1
Hans Karrer GmbH / S...	Hans Karrer Hydrocream Mi. ...	19002	3
Hans Karrer GmbH / S...	Hans Karrer Hydrocream Mi. ...	200002	1
Hans Karrer GmbH / S...	Hans Karrer Hydrocream Mi. ...	20004	1

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Supplier	Substance	Batch	Spectra
Hans Karrer GmbH /107	Hans Karrer Hydrocream Mi...	L0T19001	1
Hans Karrer GmbH	Hans Karrer Hydrocream Mi...	22002	2
Hans Karrer	Hans Karrer Hydrocream Mi...	21001	2
Hans Karrer	Hans Karrer Hydrocream Mi...	21003	2
Hans Karrer	Hans Karrer Hydrocream Mi...	21004	1
Hans Karrer	Hans Karrer Hydrocream Mi...	21005	1
Hans Karrer	Hans Karrer Hydrocream Mi...	L0T20005	1
Hans Karrer/Alliance	Hans Karrer Hydrocream Mi...	18003	2
Hans Karrer/Phönix	Hans Karrer Hydrocream Mi...	18001	1
hans Karrer/phönix	Hans Karrer Hydrocream Mi...	18003	1
Hans Karrer/Phönix	Hans Karrer Hydrocream Mi...	18003	4
Hans Karrer/Phönix	Hans Karrer Hydrocream Mi...	18004	2
Hans Karrer/Phönix	Hans Karrer Hydrocream Mi...	19001	5
Hans Karrer/Phönix	Hans Karrer Hydrocream Mi...	19003	3
Hans Karrer/Phönix	Hans Karrer Hydrocream Mi...	20001	1
Hans Karrer/Phönix	Hans Karrer Hydrocream Mi...	20005	1
Hans Karrer/Sanacorp	Hans Karrer Hydrocream Mi...	21002	1
Hans Karrer/Sanacorp	Hans Karrer Hydrocream Mi...	21004	1
Hans-Karrer GmbH	Hans Karrer Hydrocream Mi...	18003	1
hanskarrer / Gehe	Hans Karrer Hydrocream Mi...	18001	1
Hanskarrer / Gehe	Hans Karrer Hydrocream Mi...	18002	1
Hanskarrer / Gehe	Hans Karrer Hydrocream Mi...	18003	1
Hanskarrer / Gehe	Hans Karrer Hydrocream Mi...	18004	1
hanskarrer	Hans Karrer Hydrocream Mi...	19004	1
HansKarrer/Krieger	Hans Karrer Hydrocream Mi...	19003	1
HansKarrerGmbH/Phoekd	Hans Karrer Hydrocream Mi...	20004	1
Hedinger/Noweda	Sebexol® cream lotion	18424115	1
Holdermann	Sebexol® basic pH 5 formu...	1307	1
Ichthyol Gesellschaft...	Sebexol® cream lotion	1836105	1
Ichthyol	Sebexol® basic pH 5 formu...	1232	2
infectopharm/Alliance	Sebexol® cream lotion	1817227/04	1
Jäger/Noweda	Hans Karrer Hydrocream Mi...	21003	1
Jenne	Hans Karrer Hydrocream Mi...	19001	1
Karrer	Hans Karrer Hydrocream Mi...	21005	1
Karrer/Noweda	Hans Karrer Hydrocream Mi...	21003	1
Karrer/Phönix	Hans Karrer Hydrocream Mi...	18004	1
Karrer/Phönix	Hans Karrer Hydrocream Mi...	19001	1
Kehr 14.08.2020	Sebexol® cream lotion	2009227	1
Kehr	Sebexol® basic pH 5 formu...	2427103	3
kehr	Sebexol® basic pH 5 formu...	2436104	4
Kehr	Sebexol® cream lotion	2436105	1
Kehr/ Devesa	Sebexol® basic pH 5 formu...	1644102	1
Kehr/ Devesa	Sebexol® basic pH 5 formu...	1746116	4
Kehr/Devesa	Sebexol® basic pH 5 formu...	1817126	2
Kehr/Devesa	Sebexol® basic pH 5 formu...	1828110	2
Kesla Pharma Wolfen GmbH	Wofacutan wash lotion	1198201025	1
Kesla Pharma/Noweda	Wofacutan wash lotion		5
Kesla Pharma/Phönix	Wofacutan wash lotion	23819	2
Kesla Pharma/Phönix	Wofacutan wash lotion	58118	1
Kesla/Noweda	Wofacutan wash lotion		4
Leo- Pharm	Sebexol® cream lotion	1828111	1
Max Weber Apotheke	Sebexol® cream lotion	2009227	1
Nestlé Skin Health /...	Excipial® U Hydrolotio	324614	1
Nestlé Skin Health	Excipial® U Hydrolotio	315815	1
Nestlé Skin Health	Excipial® U Hydrolotio	331554	1
Nestle Skin Health/ ...	Excipial® U Hydrolotio	324614	1
Nestle Skin Health/ ...	Excipial® U Hydrolotio	331554	1
Nestlé Skin Health/Gehe	Excipial® U Hydrolotio	324614	1

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Supplier	Substance	Batch	Spectra
Nestle Skinhealth/Gehe	Excipial [®] U Hydrolotio	172481	2
Nestle Skinhealth/Gehe	Excipial [®] U Hydrolotio	173466	1
Nestle Skinhealth/Gehe	Excipial [®] U Hydrolotio	306123	2
Nestle Skinhealth/Sana	Excipial [®] U Hydrolotio	312920	2
Nestle/ Phönix	Excipial [®] U Hydrolotio	331554	2
Netslé Skin Health/Gehe	Excipial [®] U Hydrolotio	324614	1
Noweda / Dewesa	Sebexol [®] basic pH 5 formu. ...	1719111	1
NOWEDA / HERSTELLER:...	Sebexol [®] cream lotion		1
Noweda / Devesa	Sebexol [®] basic pH 5 formu. ...	1644102	3
Noweda	Sebexol [®] basic pH 5 formu. ...	1328	1
Noweda	Sebexol [®] cream lotion	1651120	1
Noweda	Sebexol [®] cream lotion	1708120	1
Noweda	Sebexol [®] cream lotion	1712223	1
Noweda	Sebexol [®] cream lotion	1802108	1
Noweda	Sebexol [®] cream lotion	1817227	1
Noweda	Sebexol [®] cream lotion	1828111	1
Noweda	Sebexol [®] cream lotion	1836105	2
Noweda	Hans Karrer Hydrocream Mi. ...	19003	1
Noweda	Sebexol [®] cream lotion	1901102	1
Noweda	Sebexol [®] cream lotion	1901103	1
Noweda	Sebexol [®] cream lotion	1912119	1
Noweda	Sebexol [®] cream lotion	1912120	1
Noweda	Sebexol [®] cream lotion	1923108	1
Noweda	Sebexol [®] cream lotion	1925121	2
Noweda	Sebexol [®] cream lotion	1947118	1
Noweda	Sebexol [®] cream lotion	1947119	3
Noweda	Sebexol [®] cream lotion	2004120	1
noweda	Sebexol [®] basic pH 5 formu. ...	2009126	1
Noweda	Sebexol [®] cream lotion	2019107	1
Noweda	Sebexol [®] cream lotion	2019207	1
Noweda	Sebexol [®] basic pH 5 formu. ...	2031128	1
Noweda	Sebexol [®] cream lotion	2040130	1
Noweda	Sebexol [®] cream lotion	2046109	1
Noweda	Hans Karrer Hydrocream Mi. ...	22002/2308232	1
Noweda	Hans Karrer Hydrocream Mi. ...	22005/2308293	1
Noweda	Sebexol [®] cream lotion	2316118	2
Noweda	Sebexol [®] cream lotion	2316119	1
Noweda	Sebexol [®] cream lotion	2316119/2311140	1
Noweda	Sebexol [®] cream lotion	2338120	2
noweda	Sebexol [®] cream lotion	2414103	1
Noweda	Sebexol [®] cream lotion	2427103	5
noweda	Sebexol [®] cream lotion	2436106	1
Noweda	Sebexol [®] cream lotion	2436106	1
Noweda	Sebexol [®] cream lotion	2513124	1
Noweda	Excipial [®] U Hydrolotio	394125	1
Noweda	Hans Karrer Hydrocream Mi. ...	LOT19001	1
Noweda	Excipial [®] U Hydrolotio	S061	1
Noweda/Devesa	Sebexol [®] cream lotion	1530	1
Noweda/Devesa	Sebexol [®] cream lotion	1605201	1
Noweda/Devesa	Sebexol [®] cream lotion	1638124	1
Noweda/Devesa	Sebexol [®] cream lotion	1720115	1
Noweda/Devesa	Sebexol [®] cream lotion	1812123	1
Noweda/devesa	Sebexol [®] cream lotion	1836106	1
Noweda/devesa	Sebexol [®] cream lotion	1923108	1
Noweda/Devesa	Sebexol [®] cream lotion	1923108	1
Noweda/devesa	Sebexol [®] cream lotion	1925121	1
Noweda/devesa	Sebexol [®] cream lotion	1947118	3

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Supplier	Substance	Batch	Spectra
Noweda/Devesa	Sebexol [®] basic pH 5 formu...	2x1407	1
Phoenix	Sebexol [®] basic pH 5 formu...	1440	1
Phoenix/Devesa	Sebexol [®] basic pH 5 formu...	1215	1
Phoenix/Devesa	Sebexol [®] basic pH 5 formu...	1407	1
Phoenix/Devesa	Sebexol [®] basic pH 5 formu...	1604127	1
Phoenix/Devesa	Sebexol [®] cream lotion	1736105	1
Phoenix/Devesa	Sebexol [®] cream lotion	1812123	1
Phoenix/Spirig	Excipial [®] U Hydrolotio	M016	1
Phönix / Devesa	Sebexol [®] basic pH 5 formu...	1644102	1
Phönix / Hans Karrer	Hans Karrer Hydrocream Mi...	20001	2
Phönix Gotha	Wofacutan wash lotion	97913	1
Phönix, Devesa, 29.0...	Sebexol [®] basic pH 5 formu...	2009126	1
Phönix, Galderma, 09...	Excipial [®] U Hydrolotio	317160	1
Phönix	Sebexol [®] basic pH 5 formu...	1313	2
Phönix	Sebexol [®] basic pH 5 formu...	1416	1
Phönix	Sebexol [®] basic pH 5 formu...	1425	2
Phönix	Sebexol [®] cream lotion	1604129	1
Phönix	Sebexol [®] cream lotion	160422	1
Phönix	Sebexol [®] cream lotion	1828111	2
Phönix	Sebexol [®] cream lotion	1912120	1
Phönix	Sebexol [®] cream lotion	1935227	1
Phönix	Sebexol [®] cream lotion	2004120	2
Phönix	Sebexol [®] cream lotion	2009227	1
phönix	Sebexol [®] cream lotion	2127108	1
Phönix	Sebexol [®] cream lotion	2128112	2
Phönix	Sebexol [®] cream lotion	2128114	2
Phönix	Sebexol [®] cream lotion	2149110	3
Phönix	Excipial [®] U Hydrolotio	331554	1
Phönix	Sebexol [®] cream lotion	4217A-03872	1
PHÖNIX	Excipial [®] U Hydrolotio	50593	1
PHÖNIX	Excipial [®] U Hydrolotio	V051	1
Phönix/ Devesa, 14.1...	Sebexol [®] basic pH 5 formu...	1935126	3
Phönix/Devesa	Sebexol [®] cream lotion	1651121	1
Phönix/Devesa	Sebexol [®] cream lotion	1712123	1
Phönix/Devesa	Sebexol [®] cream lotion	1712223	2
Phönix/Devesa	Sebexol [®] cream lotion	1812123	1
Phönix/Devesa	Sebexol [®] cream lotion	1817227	2
Phönix/Devesa	Sebexol [®] cream lotion	1824115	3
Phönix/Devesa	Sebexol [®] cream lotion	182811	1
Phönix/Devesa	Sebexol [®] cream lotion	1836105	1
Phönix/Devesa	Sebexol [®] cream lotion	1912120	1
Phönix/DEVESA	Sebexol [®] cream lotion	1935127	1
Phönix/Devesa	Sebexol [®] cream lotion	1935227	2
Phönix/Devesa	Sebexol [®] cream lotion	2019107	1
Phönix/Devesa	Sebexol [®] cream lotion	2046109	1
Phönix/Devesa	Sebexol [®] cream lotion	2103120	1
Römerapo.	Sebexol [®] cream lotion	1828110	1
Rondell Apotheke	Sebexol [®] cream lotion	1523	1
Sana / Devesa	Sebexol [®] cream lotion	2127208	1
Sana/Devesa	Sebexol [®] cream lotion	1935127	1
Sanacorp / Devesa	Sebexol [®] cream lotion	1836106	1
sanacorp, 27.9.16,4,312EUR	Sebexol [®] cream lotion	1604328	1
Sanacorp	Sebexol [®] basic pH 5 formu...	1313	1
SANACORP	Excipial [®] U Hydrolotio	172141	1
Sanacorp	Sebexol [®] cream lotion	2124116	1
Sanacorp	Sebexol [®] cream lotion	2127208	2

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Supplier	Substance	Batch	Spectra
Sanacorp	Sebexol [®] cream lotion	2128114	1
Sanacorp	Sebexol [®] cream lotion	2316119	2
Sanacorp	Sebexol [®] basic pH 5 formu. ...	2337114	2
Sanacorp	Sebexol [®] cream lotion	2338120	2
Sanacorp	Sebexol [®] basic pH 5 formu. ...	2427103	1
SANACORP/Devasa	Sebexol [®] cream lotion	1947119	1
Sanacrp	Sebexol [®] cream lotion	2436105	1
Sebexol	Sebexol [®] basic pH 5 formu. ...	1313	1
Sebexol	Sebexol [®] basic pH 5 formu. ...	1333	1
Sebexol	Sebexol [®] cream lotion	1604129	1
Sebexol	Sebexol [®] cream lotion	1812123	1
Sebexol/ Noweda	Sebexol [®] basic pH 5 formu. ...	1403	1
Sebexol/ Noweda	Sebexol [®] basic pH 5 formu. ...	1430	1
Sebexol/AHD	Sebexol [®] basic pH 5 formu. ...	1303	2
Spirig Pharma AG/ NOWEDA	Excipial [®] U Hydrolotio	LOTN022	1
Spirig Pharma AG/Noweda	Excipial [®] U Hydrolotio	R054	1
Spirig Pharma	Excipial [®] U Hydrolotio	N033	1
Spirig	Excipial [®] U Hydrolotio	N013	1
Spirig	Excipial [®] U Hydrolotio	N013	1
Spirig/Gehe	Excipial [®] U Hydrolotio	R054	3
Taosis	Sebexol [®] cream lotion	1828110	1
THC Pharma	Sebexol [®] cream lotion	1727107	1

- 18 833 spectra from 1547 *Apo-Ident* customers from a total of 6042 batches from a further 160 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Sebexol[®]/Wofacutan/Hans Karrer/Excipial* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sebexol[®]/Wofacutan/Hans Karrer/Excipial* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	1375	0	26 559
Type B	0	730	25	30 108
Type C	0	1942	3	18 641

The substance/substance group *Sebexol[®]/Wofacutan/Hans Karrer/Excipial* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9613 %)	100.0000 % (> 99.5636 %)
Type B	100.0000 % (> 99.9565 %)	96.6887 % (> 96.2914 %)
Type C	100.0000 % (> 99.0497 %)	99.8458 % (> 99.6915 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30731	30731	0.00	40.12
30839	30839	0.00	37.49
30972	30972	0.00	40.75
31065	31065	0.00	38.23
31073	31073	0.00	36.53
31103	31103	0.00	34.76
31104	31104	0.00	38.21
31279	31279	0.00	38.15
31495	31495	0.00	21.13
31509	31509	0.00	33.13
31536	31536	0.00	36.61
31592	31592	0.00	35.47
31628	31628	0.00	32.84
31839	31839	0.00	34.19
31958	31958	0.00	22.17
31961	31961	0.00	36.01
32743	32743	0.00	30.13
32744	32744	0.00	31.68
33190	33190	0.00	39.66
33191	33191	0.00	39.65
33483	33483	0.00	35.30
33502	33502	0.00	33.66
33789	33789	0.00	20.77
34116	34116	0.00	42.16
35469	35469	0.00	34.09
36726	36726	0.00	44.51
36727	36727	0.00	44.46
36764	36764	0.00	34.40
36768	36768	0.00	38.91
36773	36773	0.00	32.31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Siam benzoin (solution)**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31490-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Siam benzoin (solution)

Special notes

When selecting the *Siam benzoin (solution)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Siam benzoin (solution)	4	2	0

Second-stage model

For differentiation of the substance/substance group *Siam benzoin (solution)* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Siam benzoin (solution)* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cinnamon bark oil, Ceylon	112.79	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Siam benzoin (solution)* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Siam benzoin (solution)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Siam benzoin (solution)	3602151	31490	60	not required
Primavera	Siam benzoin (solution)	00051M23	31844	60	not required
Primavera	Siam benzoin (solution)	00074M26	34388	40	not required
Primavera	Siam benzoin (solution)	00483E31	37781	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 4 reference samples from the substance/substance group *Siam benzoin (solution)*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 734 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by

this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Siam benzoin (solution)*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Siam benzoin (solution)	00218C24	32184	40
Primavera	Siam benzoin (solution)	00606B26	34171	40

- 30 850 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Siam benzoin (solution)*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 20 778 spectra from 1559 *Apo-Ident* customers from a total of 6352 batches from a further 167 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Siam benzoin (solution)* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Siam benzoin (solution)* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	80	0	30 850
Type C	0	0	0	20 778

The substance/substance group *Siam benzoin (solution)* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0752 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31490	31490	0.00	112.79
31844	31844	0.00	208.70
34388	34388	0.00	241.78
37781	37781	0.00	234.97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Spearmint oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30453-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Spearmint oil; Oleum mentha spicata

Special notes

When selecting the *Spearmint oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Spearmint oil	4	1	6

Second-stage model

For differentiation of the substance/substance group *Spearmint oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Spearmint oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Juniper berry oil	41.34	—
Angelica root oil	43.87	—
Dwarf pine oil	45.76	—
Bergamot oil	52.88	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Spearmint oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Spearmint oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Spearmint oil	33894-111575BAG90451	31135	30	not required
Taoasis	Spearmint oil	946-120296	31685	60	not required
Taoasis	Spearmint oil	421012-129111	33481	40	not required
Taoasis	Spearmint oil	18061	38596	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 170 spectra of 4 reference samples from the substance/substance group *Spearmint oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.

- 27764 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Spearmint oil*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Spearmint oil	421012-126408	33200	40
Taoasis	Spearmint oil	421012-126408	33201	40

- 30850 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 3 *Apo-Ident* customers from 6 batches from the substance/substance group *Spearmint oil*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Spearmint oil	106765-15254	1
Taoasis	Spearmint oil	106555-5139	1
Taoasis	Spearmint oil	106555-973	1
Taoasis	Spearmint oil	27537-96244	1
Taoasis	Spearmint oil	421012-123260	1
Taoasis	Spearmint oil	421012-125373	1

- 20772 spectra from 1559 *Apo-Ident* customers from a total of 6346 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

mented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Spearmint oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Spearmint oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	170	0	27 764
Type B	0	80	0	30 850
Type C	0	6	0	20 772

The substance/substance group *Spearmint oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 96.4706 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0666 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31135	31135	0.00	54.73
31685	31685	0.00	57.32
33481	33481	0.00	47.81
38596	38596	0.00	55.91

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Spruce needle oil / Pine silvestris oil / Frankincense oil / Silver**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31032-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Spruce needle oil / Pine silvestris oil / Frankincense oil / Silver fir oil; Frankincense oil; Oleum abies alba; Oleum boswellia serrata; Oleum pini sibiricum; Oleum pini silvestris; Pine silvestris oil; Silver fir oil; Spruce needle oil

Special notes

When selecting the *Spruce needle oil / Pine silvestris oil / Frankincense oil / Silver fir oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Spruce needle oil / Pine silvestris oil / Frankincense oil / Silver fir oil	19	12	29

Second-stage model

For differentiation of the substance/substance group *Spruce needle oil* / *Pine silvestris oil* / *Frankincense oil* / *Silver fir oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Spruce needle oil* / *Pine silvestris oil* / *Frankincense oil* / *Silver fir oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Juniper berry oil	10.62	—
Swiss pine oil	13.18	—
Angelica root oil	15.31	—
Spearmint oil	21.99	—
Dwarf pine oil	23.64	—
Ginger oil	26.88	—
Hyssop oil	28.38	—
Rosemary oil	29.32	—
Citrus oil	30.25	—
Camphor oil	30.98	—
Citric oil	32.99	—
Marjoram oil	33.63	—
Cumin oil	34.24	—
Cypress oil	34.30	—
Lime oil	38.01	—
Sage oil	39.69	—
Myrtle oil	44.87	—
Matricaria oil, morrocan	50.56	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Spruce needle oil* / *Pine silvestris oil* / *Frankincense oil* / *Silver fir oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Spruce needle oil* / *Pine silvestris oil* / *Frankincense oil* / *Silver fir oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Frankincense oil	15181-119714	31633	60	not required
Taoasis	Frankincense oil	1509-125625	33052	40	not required
Taoasis	Frankincense oil	4314-129238	33646	40	not required

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Frankincense oil	1500910-128786	33650	40	not required
Taoasis	Frankincense oil	1500910-128786	33652	40	not required
Taoasis	Frankincense oil	9205-16205	37680	40	not required
Taoasis	Frankincense oil	106677-17102	37681	40	not required
Primavera	Pine silvestris oil	00664E26	34177	40	not required
Taoasis	Pine silvestris oil	1790-129074	33815	40	not required
Taoasis	Pine silvestris oil	11361-16745	37687	40	not required
Primavera	Silver fir oil	00287M26	34391	40	not required
Taoasis	Silver fir oil	120830-111781	31032	40	not required
Taoasis	Silver fir oil	211-114751	31255	40	not required
Taoasis	Silver fir oil	01A0B15-121623	31754	60	not required
Taoasis	Silver fir oil	1.21-17364	37660	40	not required
Primavera	Spruce needle oil	00465B31	37782	40	not required
Taoasis	Spruce needle oil	1507-122520	31819	60	not required
Taoasis	Spruce needle oil	1719-124011	32066	60	not required
Taoasis	Spruce needle oil	10213-149	33726	40	not required
Taoasis	Spruce needle oil	10262-16753B	37685	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 880 spectra of 20 reference samples from the substance/substance group *Spruce needle oil* / *Pine silvestris oil* / *Frankincense oil* / *Silver fir oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 19 different batches.
- 27 054 spectra from a total of 581 batches from further 140 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 540 spectra of 13 reference samples from the substance/substance group *Spruce needle oil* / *Pine silvestris oil* / *Frankincense oil* / *Silver fir oil*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Frankincense oil	00446M26	34400	40
Taoasis	Frankincense oil	3.26550	30843	40
Taoasis	Frankincense oil	1509-122197	31820	60
Taoasis	Frankincense oil	2124-2905	34277	40
Primavera	Pine silvestris oil	00398J26	34292	40
Primavera	Pine silvestris oil	00028A27	34378	40
Taoasis	Pine silvestris oil	1790-125357BAG90451	33829	40
Taoasis	Silver fir oil	01A0B16-125623	33026	40
Caelo	Spruce needle oil	11220801	30613	40
Taoasis	Spruce needle oil	29828-103169BAG90451	30672	40
Taoasis	Spruce needle oil	1769-124969	32479	40
Taoasis	Spruce needle oil	11647-2942	34112	40
Taoasis	Silver fir oil	01A0B16-125623	33027	40

- 30 390 spectra from a total of 697 batches from further 207 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 43 spectra from 15 *Apo-Ident* customers from 30 batches from the substance/substance group *Spruce needle oil* / *Pine silvestris oil* / *Frankincense oil* / *Silver fir oil*.
- Among them are spectra of independent samples from 29 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Apoth.Bauer&Co/Noweda	Frankincense oil		1
Apoth.Bauer&Co/Noweda	Frankincense oil	3175391505	1
Apotheker Bauer	Frankincense oil	1234567	1
Caelo	Spruce needle oil	10185604	1
Caelo	Spruce needle oil	11324401	4
Caelo	Spruce needle oil	13152001	2
Primavera	Spruce needle oil	1670814	1
Taoasis GmbH	Pine silvestris oil	2654-8453	1
Taoasis GmbH	Spruce needle oil	51093-10636	1
Taoasis	Spruce needle oil	114780-6023	2
Taoasis	Spruce needle oil	11647-1921	3
Taoasis	Spruce needle oil	1769-124949	1
Taoasis	Spruce needle oil	1769-124969	2
Taoasis	Spruce needle oil	1769-127000	2
Taoasis	Pine silvestris oil	1940-5617	1
Taoasis	Pine silvestris oil	1940-6527	1
Taoasis	Silver fir oil	212-120342	1
Taoasis	Silver fir oil	2507-7785	1
Taoasis	Spruce needle oil	2603-8127	1
Taoasis	Spruce needle oil	2623-8447	1
Taoasis	Pine silvestris oil	2654-8453	2
Taoasis	Spruce needle oil	29828-107964	1
Taoasis	Silver fir oil	30447-125444	1
Taoasis	Spruce needle oil	442-113922	1
Taoasis	Spruce needle oil	51093-10636	1
Taoasis	Spruce needle oil	534374-22869	1

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Supplier	Substance	Batch	Spectra
Taoasis	Spruce needle oil	534474-111585	1
Taoasis	Frankincense oil	549702-112299	1
Taoasis	Silver fir oil	C100S-10426	2
Taoasis/Sanacorp	Spruce needle oil	11647-2942	1
Taoasis/Sanacorp	Spruce needle oil	534474-111869	1
Taoasis/Sanacorp	Spruce needle oil	534474-113171	1

- 20 735 spectra from 1559 *Apo-Ident* customers from a total of 6323 batches from a further 163 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Spruce needle oil* / *Pine silvestris oil* / *Frankincense oil* / *Silver fir oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Spruce needle oil* / *Pine silvestris oil* / *Frankincense oil* / *Silver fir oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	880	0	27 054
Type B	0	443	97	30 390
Type C	0	30	13	20 735

The substance/substance group *Spruce needle oil* / *Pine silvestris oil* / *Frankincense oil* / *Silver fir oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9613 %)	100.0000 % (> 99.3182 %)
Type B	100.0000 % (> 99.9564 %)	82.0370 % (> 81.4815 %)
Type C	100.0000 % (> 99.0594 %)	69.7674 % (> 62.7907 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31032	31032	0.00	32.65
31255	31255	0.00	34.86
31633	31633	0.00	79.49
31754	31754	0.00	21.15
31819	31819	0.00	16.85
32066	32066	0.00	18.70
33052	33052	0.00	32.01
33646	33646	0.00	13.59
33650	33650	0.00	90.27
33652	33652	0.00	88.26
33726	33726	0.00	13.18
33815	33815	0.00	15.77
34177	34177	0.00	20.67
34391	34391	0.00	28.50
37660	37660	0.00	18.43
37680	37680	0.00	85.61
37681	37681	0.00	24.70
37685	37685	0.00	13.28
37687	37687	0.00	19.18
37782	37782	0.00	28.38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Strawberry aroma**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30643-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Strawberry aroma; Strawberry flavour

Special notes

When selecting the *Strawberry aroma* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Strawberry aroma	4	4	55

Second-stage model

For differentiation of the substance/substance group *Strawberry aroma* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Strawberry aroma* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Raspberry aroma	41.89	–
Contramarum aroma	82.68	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Strawberry aroma* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Strawberry aroma*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Strawberry aroma	11178804	30643	40	1402439
Caelo	Strawberry aroma	13252407	31395	40	not required
Caelo	Strawberry aroma	15411807	32814	40	not required
Caelo	Strawberry aroma	15411807	32838	40	1704074
Caelo	Strawberry aroma	23000260001	36891	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Strawberry aroma*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 734 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this

entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 5 reference samples from the substance/substance group *Strawberry aroma*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Strawberry aroma	14311215	32567	40
Caelo	Strawberry aroma	170246	33056	40
Caelo	Strawberry aroma	180832	34077	40
Caelo	Strawberry aroma	192763004	35142	40
Caelo	Strawberry aroma	14311215	32837	40

- 30 730 spectra from a total of 705 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 232 spectra from 128 *Apo-Ident* customers from 58 batches from the substance/substance group *Strawberry aroma*.
- Among them are spectra of independent samples from 55 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Strawberry aroma	22002985	1
	Strawberry aroma	22002985005	4
	Strawberry aroma	22002985007	1
	Strawberry aroma	22002985008	1
	Strawberry aroma	23000260001	7
	Strawberry aroma	23000260002	1
	Strawberry aroma	23000260005	7
	Strawberry aroma	23000260012	2
Caelo	Strawberry aroma	10184917	1
Caelo	Strawberry aroma	10803202	1

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Supplier	Substance	Batch	Spectra
Caelo	Strawberry aroma	11178813	1
Caelo	Strawberry aroma	12183504	2
Caelo	Strawberry aroma	12183511	1
Caelo	Strawberry aroma	12183513	4
Caelo	Strawberry aroma	13252405	1
Caelo	Strawberry aroma	13252407	2
Caelo	Strawberry aroma	13252409	2
Caelo	Strawberry aroma	13252417	1
Caelo	Strawberry aroma	14311204	1
Caelo	Strawberry aroma	14311209	6
Caelo	Strawberry aroma	14311215	2
Caelo	Strawberry aroma	15411805	7
Caelo	Strawberry aroma	15411807	4
Caelo	Strawberry aroma	15411813	4
Caelo	Strawberry aroma	17024604	6
Caelo	Strawberry aroma	17024606	7
Caelo	Strawberry aroma	17024607	1
Caelo	Strawberry aroma	17024608	7
Caelo	Strawberry aroma	180083208	1
Caelo	Strawberry aroma	18083202	8
Caelo	Strawberry aroma	18083206	4
Caelo	Strawberry aroma	18083208	4
Caelo	Strawberry aroma	18083211	4
Caelo	Strawberry aroma	18083214	5
Caelo	Strawberry aroma	18083215	5
Caelo	Strawberry aroma	192763001	2
Caelo	Strawberry aroma	192763002	6
Caelo	Strawberry aroma	192763004	2
Caelo	Strawberry aroma	192763005	5
Caelo	Strawberry aroma	192763008	3
Caelo	Strawberry aroma	192763009	3
Caelo	Strawberry aroma	192763012	4
Caelo	Strawberry aroma	192763015	7
Caelo	Strawberry aroma	197263012	2
Caelo	Strawberry aroma	21002299001	4
Caelo	Strawberry aroma	21002299004	3
Caelo	Strawberry aroma	21002299007	3
Caelo	Strawberry aroma	21002299012	1
Caelo	Strawberry aroma	21002299013	2
Caelo	Strawberry aroma	22002985001	8
Caelo	Strawberry aroma	22002985004	1
Caelo	Strawberry aroma	22002985006	1
Caelo	Strawberry aroma	70441927634	1
Caelo	Strawberry aroma	9101405	1
Caesar & Loretz GmbH...	Strawberry aroma	18083206	1
Caesar & Loretz GmbH...	Strawberry aroma	23000260001	1
Caesar & Loretz GmbH	Strawberry aroma	18083208	1
Caesar & Loretz GmbH	Strawberry aroma	18083211	3
Caesar & Loretz GmbH	Strawberry aroma	18083215	1
Caesar & Loretz GmbH	Strawberry aroma	192763002	1
Caesar & Loretz GmbH	Strawberry aroma	192763004	1
Caesar & Loretz GmbH	Strawberry aroma	192763008	1
Caesar & Loretz GmbH	Strawberry aroma	192763015	1
Caesar & Loretz GmbH	Strawberry aroma	21002299007	6
Caesar & Loretz GmbH	Strawberry aroma	21002299010	1
Caesar & Loretz GmbH	Strawberry aroma	21002299012	1
Caesar & Loretz GmbH	Strawberry aroma	21002299013	1
Caesar & Loretz GmbH	Strawberry aroma	22002985001	6
Caesar & Loretz GmbH	Strawberry aroma	22002985002	1
Caesar & Loretz GmbH	Strawberry aroma	22002985005	2

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Strawberry aroma	22002985007	2
Caesar & Loretz GmbH...	Strawberry aroma	18083206	1
Caesar & Loretz GmbH...	Strawberry aroma	192763008	1
Caesar & Loretz GmbH/AHD	Strawberry aroma	192763008	1
Caesar & Loretz GmbH/Gehe	Strawberry aroma	192763016	1
Caesar & Loretz GmbH/Gehe	Strawberry aroma	22002985001	2
Caesar & Loretz GmbH/Gehe	Strawberry aroma	23000260001	1
Caesar & Loretz GmbH...	Strawberry aroma	18083211	2
Caesar & Loretz GmbH...	Strawberry aroma	192763008	1
Caesar&Lorenz	Strawberry aroma	192763004	1
Caleo	Strawberry aroma	14311209	1
Erdbeer-Aroma	Strawberry aroma	17024608	1
Gehe	Strawberry aroma	17024606	1
Gehe	Strawberry aroma	192763002	1
Gehe	Strawberry aroma	23000260005	2
Hedinger	Strawberry aroma	14311215	1
Kehr	Strawberry aroma	21002299005	3
noweda	Strawberry aroma	192763002	1
Noweda	Strawberry aroma	21002299013	1
Noweda	Strawberry aroma	22002985007	1
Sanacorp	Strawberry aroma	18083211	1
Sanacorp	Strawberry aroma	22002985007	1

- 20 546 spectra from 1555 *Apo-Ident* customers from a total of 6294 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Strawberry aroma* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Strawberry aroma* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	200	0	27 734
Type B	0	200	0	30 730
Type C	0	232	0	20 546

The substance/substance group *Strawberry aroma* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.0584 %)	100.0000 % (> 97.4138 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30643	30643	0.00	85.25
31395	31395	0.00	71.59
32814	32814	0.00	81.14
32838	32838	0.00	60.51
36891	36891	0.00	82.60

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Swiss pine oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31553-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Swiss pine oil; Oleum pinus cembra

Special notes

When selecting the *Swiss pine oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Swiss pine oil	5	3	3

Second-stage model

For differentiation of the substance/substance group *Swiss pine oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Swiss pine oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Angelica root oil	11.60	—
Frankincense oil	13.12	—
Dwarf pine oil	14.29	—
Silver fir oil	19.27	—
Cypress oil	20.20	—
Pine silvestris oil	20.51	—
Spruce needle oil	21.00	—
Juniper berry oil	25.90	—
Spearmint oil	28.98	—
Ginger oil	30.39	—
Marjoram oil	31.93	—
Cumin oil	32.89	—
Citus oil	35.21	—
Tea tree oil	44.73	—
Camphor oil	53.87	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Swiss pine oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Swiss pine oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Swiss pine oil	4892-117271	31553	60	not required
Taoasis	Swiss pine oil	3023-120087	31680	60	not required
Taoasis	Swiss pine oil	12069-127103	32934	40	not required
Taoasis	Swiss pine oil	10304-128929	33645	40	not required
Taoasis	Swiss pine oil	PC121-16660	37677	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Swiss pine oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 694 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Swiss pine oil*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Swiss pine oil	00661A27	34386	40
Primavera	Swiss pine oil	00509L31	37975	40
Taoasis	Swiss pine oil	201610159-126370	32793	40

- 30 810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Swiss pine oil*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Swiss pine oil	PC121-16660	1
Caelo	Swiss pine oil	6158653	1
Oswald	Swiss pine oil	9971217	1
Taoasis	Swiss pine oil	2552-7162	1

- 20 774 spectra from 1559 *Apo-Ident* customers from a total of 6348 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Swiss pine oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Swiss pine oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	240	0	27 694
Type B	0	80	40	30 810
Type C	0	4	0	20 774

The substance/substance group *Swiss pine oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9566 %)	66.6667 % (> 64.1667 %)
Type C	100.0000 % (> 99.0708 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31553	31553	0.00	12.95
31680	31680	0.00	14.27
32934	32934	0.00	26.63
33645	33645	0.00	13.31
37677	37677	0.00	13.45

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Tea tree oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30959-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Tea tree oil; Oleum melaleuca alternifolia

Special notes

When selecting the *Tea tree oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tea tree oil	4	5	32

Second-stage model

For differentiation of the substance/substance group *Tea tree oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tea tree oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	21.01	—
Carrot seed oil	49.71	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tea tree oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Tea tree oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Tea tree oil	533902-109942BAG91303	30959	40	not required
Taoasis	Tea tree oil	34828-113642BAG91303	31134	40	not required
Taoasis	Tea tree oil	44737-121997	31762	60	not required
Taoasis	Tea tree oil	20015	38774	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Tea tree oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 754 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are

listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 5 reference samples from the substance/substance group *Tea tree oil*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Tea tree oil	00667A27	34396	40
Primavera	Tea tree oil	00194J31	37784	40
Taoasis	Tea tree oil	52642-125539	33017	40
Taoasis	Tea tree oil	52642-124527	33018	40
Taoasis	Tea tree oil	17186AUR08	37772	40

- 30 730 spectra from a total of 704 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 51 spectra from 17 *Apo-Ident* customers from 32 batches from the substance/substance group *Tea tree oil*.
- Among them are spectra of independent samples from 32 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tea tree oil	18536(AU)	1
	Tea tree oil	P412024	1
Bergland/Anzag	Tea tree oil	K8000627	1
Caelo	Tea tree oil	15051806	2
Caelo	Tea tree oil	15051807	1
Caelo	Tea tree oil	15337105	1
Caelo	Tea tree oil	15337106	1
Caelo	Tea tree oil	15337112	1
Caelo	Tea tree oil	365G26	1
Ferd.Eimermacher GmbH	Tea tree oil	73900719	1
Primavera, Gehe	Tea tree oil	342B26	1

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Supplier	Substance	Batch	Spectra
Taoasis	Tea tree oil	128919-AUJ07	1
Taoasis	Tea tree oil	1469-117418	2
Taoasis	Tea tree oil	20210070213651	1
Taoasis	Tea tree oil	20269-116833	2
Taoasis	Tea tree oil	20269-117745G09	1
Taoasis	Tea tree oil	28348-119841	1
Taoasis	Tea tree oil	28348-121515	1
Taoasis	Tea tree oil	28348-121597	2
Taoasis	Tea tree oil	52642-12078	1
Taoasis	Tea tree oil	52642-124559	1
Taoasis	Tea tree oil	52642-124919	1
Taoasis	Tea tree oil	52642-125539BAG91303	12
Taoasis	Tea tree oil	702-13926	1
Taoasis	Tea tree oil	76283-129307	2
Taoasis	Tea tree oil	76283-778	1
Taoasis	Tea tree oil	90725-2423	1
Taoasis	Tea tree oil	92962-3613	1
Taoasis	Tea tree oil	92962-3626	2
Taoasis	Tea tree oil	92962-5142	3
Taoasis	Tea tree oil	929626409	1
Taoasis/Taoasis	Tea tree oil	JF20461-1972	1

- 20 727 spectra from 1559 *Apo-Ident* customers from a total of 6320 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Tea tree oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tea tree oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	180	0	27 754
Type B	0	200	0	30 730
Type C	0	51	0	20 727

The substance/substance group *Tea tree oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9617 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.0592 %)	100.0000 % (> 88.2353 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30959	30959	0.00	51.20
31134	31134	0.00	52.32
31762	31762	0.00	58.01
38774	38774	0.00	45.72

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Thyme oil, red**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30929-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Thyme oil, red; Oleum thymus vulgaris

Special notes

When selecting the *Thyme oil, red* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Thyme oil, red	6	2	26

Second-stage model

For differentiation of the substance/substance group *Thyme oil, red* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Thyme oil, red* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Savory herb	11.41	—
Oregano oil	18.07	—
Marjoram oil	80.83	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Thyme oil, red* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Thyme oil, red*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Thyme oil, red	31911-109378	30929	40	not required
Taoasis	Thyme oil, red	9434-115427	31259	40	not required
Taoasis	Thyme oil, red	56081-124964	32482	40	not required
Taoasis	Thyme oil, red	1829-125364	32981	40	not required
Taoasis	Thyme oil, red	1976-2943	34103	40	not required
Taoasis	Thyme oil, red	6164-12709	35537	60	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Thyme oil, red*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 6 different batches.

- 27674 spectra from a total of 594 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Thyme oil, red*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Thyme oil, red	40517-121881	32472	40
Taoasis	Thyme oil, red	19932	38784	40

- 30850 spectra from a total of 707 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 35 spectra from 11 *Apo-Ident* customers from 27 batches from the substance/substance group *Thyme oil, red*.
- Among them are spectra of independent samples from 26 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Thyme oil, red	2302-7572	1
Caelo	Thyme oil, red	19243015	1
Caelo	Thyme oil, red	21000083004	1
Caesar & Loretz GmbH	Thyme oil, red	5841	1
Noweda/ Taoasis 07.0...	Thyme oil, red	6164-10928	1
Noweda/Taoasis	Thyme oil, red	6164-12709	1
Taoasis	Thyme oil, red	14381-117385	1
Taoasis	Thyme oil, red	1976-3100	2
Taoasis	Thyme oil, red	1976-3455	1
Taoasis	Thyme oil, red	1976-5865	1
Taoasis	Thyme oil, red	1976-5867	2

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Supplier	Substance	Batch	Spectra
Taoasis	Thyme oil, red	1976-6717	1
Taoasis	Thyme oil, red	25394-118296	1
Taoasis	Thyme oil, red	32444-118785	4
Taoasis	Thyme oil, red	33092-111620	1
Taoasis	Thyme oil, red	33635-120088	1
Taoasis	Thyme oil, red	40517-121881	2
Taoasis	Thyme oil, red	43637-122713	1
Taoasis	Thyme oil, red	43637-122852	1
Taoasis	Thyme oil, red	43637-123574	1
Taoasis	Thyme oil, red	43637-124964	1
Taoasis	Thyme oil, red	4663-7499	1
Taoasis	Thyme oil, red	4952-9584	2
Taoasis	Thyme oil, red	56081-126921	1
Taoasis	Thyme oil, red	56081-127214	1
Taoasis	Thyme oil, red	8013-13890	1
Taoasis	Thyme oil, red	9434-115525	1
Taoasis/Sanacorp	Thyme oil, red	1976-3455	1

- 20 743 spectra from 1558 *Apo-Ident* customers from a total of 6325 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Thyme oil, red* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Thyme oil, red* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	27 674
Type B	0	80	0	30 850
Type C	0	34	1	20 743

The substance/substance group *Thyme oil, red* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0596 %)	97.1429 % (> 88.5714 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30929	30929	0.00	26.31
31259	31259	0.00	22.78
32482	32482	0.00	31.72
32981	32981	0.00	21.20
34103	34103	0.00	28.43
35537	35537	0.00	23.42

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Vetiver bourbon oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31546-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Vetiver bourbon oil; Oleum vetiveria zizanoides

Special notes

When selecting the *Vetiver bourbon oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Vetiver bourbon oil	5	1	9

Second-stage model

For differentiation of the substance/substance group *Vetiver bourbon oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Vetiver bourbon oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Immortelle oil	16.32	—
Rose-geranium oil, organic	20.33	—
Myrtle oil	23.80	—
Manuka oil	24.19	—
Citus oil	27.02	—
Lemon grass oil	28.65	—
Cypress oil	28.97	—
Carrot seed oil	36.92	—
Ginger oil	37.65	—
Marjoram oil	38.99	—
Hyssop oil	40.28	—
Cumin oil	42.36	—
Patchouli oil	46.18	—
Citronella oil	48.23	—
Tea tree oil	50.33	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Vetiver bourbon oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Vetiver bourbon oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Vetiver bourbon oil	7141-116418	31546	60	not required
Taoasis	Vetiver bourbon oil	7141-119962	31684	60	not required
Taoasis	Vetiver bourbon oil	7141-128198	33647	40	not required
Taoasis	Vetiver bourbon oil	1710-48621A-11231	35143	40	not required
Taoasis	Vetiver bourbon oil	19830	38777	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Vetiver bourbon oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.
- 27 694 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Vetiver bourbon oil*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Vetiver bourbon oil	7141-124922	32810	40
Taoasis	Vetiver bourbon oil	7141-124922	33046	40

- 30 850 spectra from a total of 708 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 1 *Apo-Ident* customers from 9 batches from the substance/substance group *Vetiver bourbon oil*.
- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Taoasis	Vetiver bourbon oil	108-232	1
Taoasis	Vetiver bourbon oil	2060-1665	2
Taoasis	Vetiver bourbon oil	2060-3449	1
Taoasis	Vetiver bourbon oil	2060-5667	4
Taoasis	Vetiver bourbon oil	7141-119174	1
Taoasis	Vetiver bourbon oil	7141-122195	2
Taoasis	Vetiver bourbon oil	7141-123924	1
Taoasis	Vetiver bourbon oil	7141-124600	2
Taoasis	Vetiver bourbon oil	7141-137885	1

- 20 763 spectra from 1559 *Apo-Ident* customers from a total of 6343 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Vetiver bourbon oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Vetiver bourbon oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	240	0	27 694
Type B	0	80	0	30 850
Type C	0	15	0	20 763

The substance/substance group *Vetiver bourbon oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9567 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0616 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31546	31546	0.00	26.03
31684	31684	0.00	23.11
33647	33647	0.00	22.52
35143	35143	0.00	39.12
38777	38777	0.00	30.48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group	Water and aqueous solutions
Substance class	BR APIs & excipients, liquid/semi-solid (other)
Report date	28/04/2026
Report number	10005444-2026-04-28
Executing company	HiperScan GmbH Gerokstraße 13 01307 Dresden Germany

Relevant substance names

Water and aqueous solutions; Aloe vera gel, 10x concentrated; Aqua; Retterspitz external; SyrSpend® SF pH4 cherry aroma; SyrSpend® SF pH4 aroma free; Water

Special notes

When selecting the *Water and aqueous solutions* substance/substance group, the following information is displayed to the user:

- Advice: Currently no longer available from major pharmaceutical manufacturers. Therefore, batch maintenance is currently not possible.
- Advice for the identification of water: Preserved, purified and distilled water can not be conclusively distinguished by spectral analysis. An additional analysis of identity may be required.

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Water and aqueous solutions	21	90	607

Second-stage model

For differentiation of the substance/substance group *Water and aqueous solutions* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Water and aqueous solutions* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sebexol [®] cream lotion	20.98	—
Sebexol [®] basic pH 5 formula basis	23.11	—
Wofacutan wash lotion	31.99	—
Hans Karrer Hydrocream MicroSilver	32.91	—
Dimeticone ointment 10% SR	33.39	—
Excipial [®] U Hydrolotio	36.77	—
Amciderm [®] Base cream	43.36	—
Abitima [®] clinic face cream	46.48	—
Base cream Taoasis	50.08	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Water and aqueous solutions* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Water and aqueous solutions*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Aloe vera gel, 10x concen...	13045901	31146	40	not required
Caelo	Aloe vera gel, 10x concen...	15185503	31862	60	not required
Caelo	Aloe vera gel, 10x concen...	161922	32313	40	20160707*
Caelo	Aloe vera gel, 10x concen...	20001962	35049	40	20200702*
Retterspit...	Retterspitz external	016100	32785	40	not required
Retterspit...	Retterspitz external	017058	33430	40	not required
Retterspit...	Retterspitz external	016240	33431	40	not required
Fagron	SyrSpend [®] SF pH4 cherry aroma	1503D017	31671	60	not required

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	SyrSpend [®] SF pH4 cherry aroma	1503D017	31723	60	not required
Fagron	SyrSpend [®] SF pH4 cherry aroma	1704492/1	33787	40	not required
Fagron	SyrSpend [®] SF pH4 aroma free	1503D009	31670	60	not required
Fagron	SyrSpend [®] SF pH4 aroma free	1412D002	31722	60	not required
Fagron	SyrSpend [®] SF pH4 aroma free	19011410	35077	40	not required
Fagron	SyrSpend [®] SF pH4 aroma free	22H11-T10-099025	36745	40	not required
Fagron	SyrSpend [®] SF pH4 aroma free	24G11-T03-115196	38624	40	not required
Caelo	Water	15068701	31675	45	not required
Caelo	Water	153943	32079	40	20151215*
Caelo	Water	191968	34767	40	20190815*
Caelo	Water	20003298	35239	40	20201113*
Caelo	Water	20003299	35240	40	20201113*
Caelo	Water	20003301	35242	40	20201113*
Hedinger	Water	219066	31623	60	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1005 spectra of 22 reference samples from the substance/substance group *Water and aqueous solutions*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 21 different batches.
- 26 929 spectra from a total of 579 batches from further 139 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 2805 spectra of 92 reference samples from the substance/substance group *Water and aqueous solutions*.
- Among them are spectra of independent samples from 90 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Aloe vera gel, 10x concen. ...	17082002	33511	40
Caelo	Aloe vera gel, 10x concen. ...	181255	34342	40
Caelo	Aloe vera gel, 10x concen. ...	192411	34714	40
Caelo	Aloe vera gel, 10x concen. ...	21004007001	36048	40
Retterspitz GmbH	Retterspitz external	016179	32784	30
Retterspitz GmbH	Retterspitz external	017192	34049	40
Fagron	SyrSpend® SF pH4 cherry aroma	1503255	32738	40
Fagron	SyrSpend® SF pH4 cherry aroma	1603252/2	32842	40
Fagron	SyrSpend® SF pH4 cherry aroma	23D05-T04-104277	37412	40
Fagron	SyrSpend® SF pH4 aroma free	1704493	33501	40
Caelo	Water	153944	32081	40
Caelo	Water	153712	32083	40
Caelo	Water	162553	32895	40
Caelo	Water	162867	32896	40
Caelo	Water	163533	33176	40
Caelo	Water	170018	33177	40
Caelo	Water	172191	33578	40
Caelo	Water	172192	33579	40
Caelo	Water	172220	33580	40
Caelo	Water	172533	33741	40
Caelo	Water	172827	33742	40
Caelo	Water	172861	33743	40
Caelo	Water	172862	33744	40
Caelo	Water	172771	33745	40
Caelo	Water	171147	33977	40
Caelo	Water	172957	33978	40
Caelo	Water	180045	34136	40
Caelo	Water	181105	34137	40
Caelo	Water	181354	34139	40
Caelo	Water	182286	34243	40
Caelo	Water	181952	34244	40
Caelo	Water	192421	34765	40
Caelo	Water	20002402	35114	40
Caelo	Water	20002910	35237	40
Caelo	Water	20002911	35238	40
Caelo	Water	20003300	35241	40
Caelo	Water	20003876	35243	40
Caelo	Water	21002422	35589	50
Caelo	Water	21002423	35590	50
Caelo	Water	21002424	35591	50
Caelo	Water	21002425	35592	50
Caelo	Water	21002426	35593	50
Caelo	Water	21002427	35594	50
Caelo	Water	21003472	35988	40
Caelo	Water	21003473	35989	10
Caelo	Water	21004056	35992	40
Caelo	Water	22000150	36153	40
Caelo	Water	22001967	36454	40
Caelo	Water	22001969	36455	10
Caelo	Water	22002001	36456	10
Caelo	Water	22002002	36457	10
Caelo	Water	22003132	36789	40
Caelo	Water	22003133	36790	10
Caelo	Water	22003134	36791	10
Caelo	Water	22003903	36929	40
Caelo	Water	22003904	36930	10
Caelo	Water	22003905	36931	10
Caelo	Water	22003906	36932	10
Caelo	Water	22003907	36933	10
Caelo	Water	23000973	37472	40

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Water	23000974	37473	10
Caelo	Water	23000975	37707	10
Caelo	Water	23002633	37860	40
Caelo	Water	23002634	37861	10
Caelo	Water	23002635	37862	10
Caelo	Water	23003007	37863	40
Caelo	Water	23003008	37864	10
Caelo	Water	23003009	37865	10
Caelo	Water	23003010	37866	10
Caelo	Water	23003011	37867	10
Caelo	Water	23003012	37868	10
Caelo	Water	23003013	37869	10
Caelo	Water	23003014	37870	10
Caelo	Water	24001528	38539	40
Caelo	Water	24001583	38540	10
Caelo	Water	24002031	38689	40
Caelo	Water	24002033	38691	10
Caelo	Water	24002035	38693	40
Caelo	Water	24002106	38695	40
Caelo	Water	24002357	38697	40
Caelo	Water	24002359	38699	10
Caelo	Water	24002931	38817	40
Caelo	Water	24002933	38818	10
Caelo	Water	24002934	38819	10
Caelo	Water	25000321	39013	40
Caelo	Water	25000322	39014	10
Caelo	Water	25000323	39015	10
Caelo	Water	25000510	39016	10
Caelo	Water	25000824	39021	40
Caelo	Water	25000825	39022	10
Fagron	SyrSpend [®] SF pH4 aroma free	1704493	33631	40
Caelo	Water	15068701	31675 [†]	15

- 28 125 spectra from a total of 618 batches from further 206 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3123 spectra from 649 *Apo-Ident* customers from 634 batches from the substance/substance group *Water and aqueous solutions*.
- Among them are spectra of independent samples from 599 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	SyrSpend [®] SF pH4 aroma free		1
	SyrSpend [®] SF pH4 aroma free	116-106100	1

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[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

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Supplier	Substance	Batch	Spectra
	SyrSpend [®] SF pH4 aroma free	13359062	1
	SyrSpend [®] SF pH4 aroma free	20009273	1
	SyrSpend [®] SF pH4 aroma free	21005761	2
	SyrSpend [®] SF pH4 aroma free	21009136	2
	SyrSpend [®] SF pH4 cherry aroma	21010483	2
	SyrSpend [®] SF pH4 cherry aroma	2103078	1
	SyrSpend [®] SF pH4 cherry aroma	22/14-T22-099449	1
	SyrSpend [®] SF pH4 aroma free	22000887	10
	Aloe vera gel, 10x concen. . .	22001489004	1
	SyrSpend [®] SF pH4 aroma free	2200887	1
	SyrSpend [®] SF pH4 cherry aroma	22C13-T06-103720	1
	SyrSpend [®] SF pH4 aroma free	22D11-09-095898	1
	SyrSpend [®] SF pH4 aroma free	22D11-T08-095894	1
	SyrSpend [®] SF pH4 aroma free	22D11-T09-095898	6
	SyrSpend [®] SF pH4 cherry aroma	22D11-T17	1
	SyrSpend [®] SF pH4 cherry aroma	22D11-T17-095910	4
	SyrSpend [®] SF pH4 cherry aroma	22D11-T17-095911	3
	SyrSpend [®] SF pH4 cherry aroma	22D11-T18-095918	2
	Water	22F13-03-097342	1
	SyrSpend [®] SF pH4 aroma free	22h11-t09	1
	SyrSpend [®] SF pH4 aroma free	22H11-T09	4
	SyrSpend [®] SF pH4 aroma free	22h11-t09-099022	1
	SyrSpend [®] SF pH4 aroma free	22H11-T09-099022	16
	SyrSpend [®] SF pH4 aroma free	22H11-T10-099025	4
	SyrSpend [®] SF pH4 cherry aroma	22H11-T11	1
	SyrSpend [®] SF pH4 cherry aroma	22H11-T11-099029	1
	SyrSpend [®] SF pH4 cherry aroma	22H11-T11-099030	1
	SyrSpend [®] SF pH4 cherry aroma	22H11-T13-099034	6
	SyrSpend [®] SF pH4 cherry aroma	22H11-T13-099035	1
	SyrSpend [®] SF pH4 cherry aroma	22H11-T18	2
	SyrSpend [®] SF pH4 cherry aroma	22H11-T18-099038	6
	SyrSpend [®] SF pH4 aroma free	22H11T10099025	1
	SyrSpend [®] SF pH4 cherry aroma	22H11T13099034	1
	SyrSpend [®] SF pH4 cherry aroma	22HT11-T13-099034	1
	SyrSpend [®] SF pH4 cherry aroma	22I14-T22-099449	3
	SyrSpend [®] SF pH4 aroma free	22J04-F02-383639	1
	SyrSpend [®] SF pH4 cherry aroma	22J14-T08	1
	SyrSpend [®] SF pH4 cherry aroma	22J14-T08-1000064	1
	SyrSpend [®] SF pH4 cherry aroma	22J14-T08-100064	4
	SyrSpend [®] SF pH4 cherry aroma	22J14-T08-100065	1
	SyrSpend [®] SF pH4 cherry aroma	22I14-T22-099449	1
	Water	23000006001	1
	Water	230418141	1
	SyrSpend [®] SF pH4 cherry aroma	23817-T02-103078	1
	SyrSpend [®] SF pH4 aroma free	23817-T03-103124	1
	SyrSpend [®] SF pH4 cherry aroma	2398472893465	1
	SyrSpend [®] SF pH4 cherry aroma	23A05-T07-102866	2
	SyrSpend [®] SF pH4 cherry aroma	23A10-T20	2
	SyrSpend [®] SF pH4 cherry aroma	23A10-T20-102143	4
	SyrSpend [®] SF pH4 cherry aroma	23A10-T20-102144	1
	SyrSpend [®] SF pH4 aroma free	23A16-T09	1
	SyrSpend [®] SF pH4 aroma free	23A16-T09-102194	3
	SyrSpend [®] SF pH4 aroma free	23A16-T09-102195	9
	SyrSpend [®] SF pH4 aroma free	23A24-T16	6
	SyrSpend [®] SF pH4 aroma free	23a24-t16-106100	1
	SyrSpend [®] SF pH4 aroma free	23a24-T16-106100	1
	SyrSpend [®] SF pH4 aroma free	23A24-T16-106100	2

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Supplier	Substance	Batch	Spectra
SyrSpend®	SF pH4 aroma free	23A24-T16-1061000	1
SyrSpend®	SF pH4 aroma free	23A24-T16-1206100	1
SyrSpend®	SF pH4 cherry aroma	23A26-T03	2
SyrSpend®	SF pH4 cherry aroma	23A26-T03-102457	13
SyrSpend®	SF pH4 cherry aroma	23A26-T05-102460	3
SyrSpend®	SF pH4 cherry aroma	23a26-to3-102457	1
SyrSpend®	SF pH4 aroma free	23B02-T16	1
SyrSpend®	SF pH4 aroma free	23B02-T16-106339	5
SyrSpend®	SF pH4 aroma free	23B02-T16-106340	7
SyrSpend®	SF pH4 aroma free	23B09	1
SyrSpend®	SF pH4 aroma free	23B09-T05	2
SyrSpend®	SF pH4 aroma free	23b09-T05-102908	1
SyrSpend®	SF pH4 aroma free	23B09-T05-102908	7
SyrSpend®	SF pH4 aroma free	23B10-T02	2
SyrSpend®	SF pH4 aroma free	23b10-t02-102920	1
SyrSpend®	SF pH4 aroma free	23B10-T02-102920	21
SyrSpend®	SF pH4 aroma free	23B10-T03-102920	1
SyrSpend®	SF pH4 cherry aroma	23B17-T02	1
SyrSpend®	SF pH4 cherry aroma	23B17-T02-103078	5
SyrSpend®	SF pH4 aroma free	23B17-T03	3
SyrSpend®	SF pH4 aroma free	23B17-t03-103124	1
SyrSpend®	SF pH4 aroma free	23B17-T03-103124	12
SyrSpend®	SF pH4 aroma free	23b17-t03-103125	1
SyrSpend®	SF pH4 aroma free	23B17-T03-103125	5
SyrSpend®	SF pH4 aroma free	23B17To3103125	1
SyrSpend®	SF pH4 aroma free	23B24-T09	1
SyrSpend®	SF pH4 aroma free	23B24-T09-103519	7
SyrSpend®	SF pH4 aroma free	23B02-T16-106340	1
SyrSpend®	SF pH4 aroma free	23BT17-T03-103125	1
SyrSpend®	SF pH4 cherry aroma	23C08-T03	4
SyrSpend®	SF pH4 cherry aroma	23C08-T03-1036709	1
SyrSpend®	SF pH4 cherry aroma	23c08-t03-103676	1
SyrSpend®	SF pH4 cherry aroma	23C08-T03-103676	23
SyrSpend®	SF pH4 cherry aroma	23C08-T04	3
SyrSpend®	SF pH4 cherry aroma	23c08-t04-103682	1
SyrSpend®	SF pH4 cherry aroma	23C08-T04-103682	5
SyrSpend®	SF pH4 cherry aroma	23C13-T06	1
SyrSpend®	SF pH4 cherry aroma	23C13-T06-103720	12
SyrSpend®	SF pH4 cherry aroma	23C13-T07	2
SyrSpend®	SF pH4 cherry aroma	23C13-T07-1037203	1
SyrSpend®	SF pH4 cherry aroma	23C13-T07-103723	8
SyrSpend®	SF pH4 cherry aroma	23C13T06103720	1
SyrSpend®	SF pH4 cherry aroma	23C08-T03-103676	1
SyrSpend®	SF pH4 cherry aroma	23D05-T03-104272	7
SyrSpend®	SF pH4 cherry aroma	23D05-T04-104277	4
SyrSpend®	SF pH4 cherry aroma	23D05-T05-099074	2
SyrSpend®	SF pH4 cherry aroma	23D05T03104272	1
SyrSpend®	SF pH4 cherry aroma	23E-T05-105417	1
SyrSpend®	SF pH4 cherry aroma	23E12-T02	2
SyrSpend®	SF pH4 cherry aroma	23E12-T02-1052407	4
SyrSpend®	SF pH4 cherry aroma	23E12-T02-105247	9
SyrSpend®	SF pH4 cherry aroma	23E12-T02	1
SyrSpend®	SF pH4 aroma free	23E19-T-105395	1
SyrSpend®	SF pH4 aroma free	23E19-T12-1053706	1
SyrSpend®	SF pH4 aroma free	23E19-T12-105376	10
SyrSpend®	SF pH4 aroma free	23E19-T12-10576	1

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Supplier	Substance	Batch	Spectra
	SyrSpend [®] SF pH4 aroma free	23E19-T15	1
	SyrSpend [®] SF pH4 aroma free	23E19-T15-1053807	1
	SyrSpend [®] SF pH4 aroma free	23e19-t15-105387	1
	SyrSpend [®] SF pH4 aroma free	23E19-T15-105387	11
	SyrSpend [®] SF pH4 aroma free	23E19-T16	1
	SyrSpend [®] SF pH4 aroma free	23E19-T16-10053900	1
	SyrSpend [®] SF pH4 aroma free	23E19-T16-105390	13
	SyrSpend [®] SF pH4 aroma free	23E19-T17	1
	SyrSpend [®] SF pH4 aroma free	23E19-T17-105395	9
	SyrSpend [®] SF pH4 aroma free	23E19T17-105395	1
	SyrSpend [®] SF pH4 cherry aroma	23E22-T05	2
	SyrSpend [®] SF pH4 cherry aroma	23E22-T05-105417	18
	SyrSpend [®] SF pH4 cherry aroma	23E22-T14	3
	SyrSpend [®] SF pH4 cherry aroma	23E22-T14-1054407	1
	SyrSpend [®] SF pH4 cherry aroma	23E22-T14-105447	3
	SyrSpend [®] SF pH4 cherry aroma	23E22-T15-1054505	1
	SyrSpend [®] SF pH4 cherry aroma	23E22-T06-105420	1
	SyrSpend [®] SF pH4 cherry aroma	23F14-T12	1
	SyrSpend [®] SF pH4 cherry aroma	23F14-T12-106215	11
	SyrSpend [®] SF pH4 aroma free	23F16-T02-106346	1
	SyrSpend [®] SF pH4 aroma free	23F19-T16-105390	1
	Water	24001055001	1
	Water	24001146001	1
	Water	24A10-T18-08968	1
	SyrSpend [®] SF pH4 aroma free	24G11-T03-115196	4
	SyrSpend [®] SF pH4 aroma free	24G11-T03-115196	1
	Water	24i25-T04-115791	1
	SyrSpend [®] SF pH4 aroma free	24K20-T02	1
	SyrSpend [®] SF pH4 aroma free	24K20-T02-117948	11
	Water	25A06-T04-117585	1
	SyrSpend [®] SF pH4 aroma free	25B07-T04	1
	SyrSpend [®] SF pH4 aroma free	25B07-T04-119651	3
	SyrSpend [®] SF pH4 cherry aroma	25G17-T05-123203	1
	SyrSpend [®] SF pH4 cherry aroma	25G17-T05-123204	1
	SyrSpend [®] SF pH4 cherry aroma	25G25-T06-124284	1
	SyrSpend [®] SF pH4 aroma free	25H21-T02	1
	Water	31344	1
	Water	33214	1
	SyrSpend [®] SF pH4 aroma free	9-09589008	1
	SyrSpend [®] SF pH4 cherry aroma	fagron	1
	SyrSpend [®] SF pH4 cherry aroma	T01-1030708	1
	SyrSpend [®] SF pH4 cherry aroma	T02-1052407	6
	SyrSpend [®] SF pH4 aroma free	T03-1151906	2
	SyrSpend [®] SF pH4 cherry aroma	T05-1054107	4
	SyrSpend [®] SF pH4 cherry aroma	T0510246000	1
	SyrSpend [®] SF pH4 cherry aroma	T07-1037203	7
	SyrSpend [®] SF pH4 aroma free	T09-1035109	1
	SyrSpend [®] SF pH4 aroma free	T12-1053706	9
	SyrSpend [®] SF pH4 cherry aroma	T13_0990304	1
	SyrSpend [®] SF pH4 cherry aroma	T14-1054407	1
	SyrSpend [®] SF pH4 aroma free	T15-1053807	8
	SyrSpend [®] SF pH4 aroma free	T16-106100	1
	SyrSpend [®] SF pH4 aroma free	T16-1061000	8
	SyrSpend [®] SF pH4 aroma free	T17-1053904	2
	SyrSpend [®] SF pH4 aroma free	T17-1053905	6
	SyrSpend [®] SF pH4 aroma free	T02-1029200	1
	SyrSpend [®] SF pH4 cherry aroma	To7_1037203	1

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Supplier	Substance	Batch	Spectra
AEP	Water	20SIB009	1
AHD	SyrSpend [®] SF pH4 aroma free	22H1-T09-099022	1
AHD	SyrSpend [®] SF pH4 aroma free	23B02-T16-106339	1
AHD	SyrSpend [®] SF pH4 aroma free	23B09-T05-102908	1
AHD	SyrSpend [®] SF pH4 aroma free	23B17-T03-103124	1
Alliance Health Care	SyrSpend [®] SF pH4 aroma free	23B17-T03-103124	1
Alliance Healthcare	SyrSpend [®] SF pH4 cherry aroma	21002532	6
Alliance	SyrSpend [®] SF pH4 cherry aroma	20004332	4
Alliance	SyrSpend [®] SF pH4 cherry aroma	20007125	8
Alliance	SyrSpend [®] SF pH4 aroma free	22H11-T09-099022	1
Alliance	SyrSpend [®] SF pH4 cherry aroma	23A26-T03-102457	1
Alliance	SyrSpend [®] SF pH4 cherry aroma	23C13-T07-103723	1
Alliance	SyrSpend [®] SF pH4 cherry aroma	23E12-T02-105247	1
Alliance	SyrSpend [®] SF pH4 aroma free	23E19-T17-105395	1
Alliance	SyrSpend [®] SF pH4 cherry aroma	23E22-T05-105417	2
Alliance	SyrSpend [®] SF pH4 cherry aroma	23E22-T05-105417	1
Anzag	SyrSpend [®] SF pH4 aroma free	19011410	1
Anzag	SyrSpend [®] SF pH4 aroma free	20004220	1
Anzag	SyrSpend [®] SF pH4 aroma free	22H11-T10-099025	2
Anzag	SyrSpend [®] SF pH4 cherry aroma	231213(23A26-T03-102457)	1
Anzag	SyrSpend [®] SF pH4 aroma free	23B02-T16	1
Anzag	SyrSpend [®] SF pH4 aroma free	23B09-T05-102908	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	23E22-T05-105417	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	240115(23A26-T03-102457)	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	240228(23A26-T03-102457)	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	240412(23A26-T03-102457)	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	240507(23A26-T03-102457)	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	240530(23A26-T03-102457)	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	240726(23A26-T03-102457)	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	241212	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	250220(23E22-T05-105417)	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	250428(23E22-T05-105417)	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	250512(23E22-T05-105417)	1
apomix	SyrSpend [®] SF pH4 cherry aroma	15C19/C	1
apomix	Water	17H24-T09-044709	1
apomix	SyrSpend [®] SF pH4 cherry aroma	1800673/1	1
Apotheke	Water	4/20	1
Audor Pharma	SyrSpend [®] SF pH4 cherry aroma	1909423/1	2
B. Braun Melsungen AG	Water	223968001	2
B.Braun Melsungen AG...	Water	18272011	1
B.Braun Melsungen AG...	Water	18264014	1
Bombastus	SyrSpend [®] SF pH4 cherry aroma	1803724/2	1
Caelo	Water		2
Caelo	Water	10038564	1
Caelo	Water	13121720	1
Caelo	Water	14IL38	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1503255	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1507318	3
Caelo	Water	151005027617	1
Caelo	Aloe vera gel, 10x concen...	15185503	1
Caelo	Aloe vera gel, 10x concen...	15185512	1
Caelo	Water	15336501	1
Caelo	Water	15394201	1
Caelo	Water	15K10-T04-027613	1
Caelo	Water	16151201	1
Caelo	Water	16211901	2
Caelo	Water	16223801	4

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Supplier	Substance	Batch	Spectra
Caelo	Water	16255101	1
Caelo	Water	16353303	1
Caelo	Water	16F13-T11-034264	1
Caelo	Water	16F13-T16-034297	1
Caelo	Water	16F13-T18-34301	1
Caelo	Water	17002001	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1702015	7
Caelo	SyrSpend [®] SF pH4 cherry aroma	1704492	1
Caelo	SyrSpend [®] SF pH4 aroma free	1704493	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1707302/1	2
Caelo	Water	17114701	3
Caelo	Water	17114801	1
Caelo	SyrSpend [®] SF pH4 aroma free	1712018	1
Caelo	SyrSpend [®] SF pH4 aroma free	1712023/2	3
Caelo	SyrSpend [®] SF pH4 cherry aroma	1712024	1
Caelo	Water	17145001	3
Caelo	Water	17149501	1
Caelo	Water	17173001	1
Caelo	Water	17211201	1
Caelo	Water	17219101	2
Caelo	Water	17277102	2
Caelo	Water	17282701	3
Caelo	Water	17295701	1
Caelo	Water	1733981	1
Caelo	Water	17B13-T04-041608	1
Caelo	Water	17K27-T10-050547	1
Caelo	Water	17K27-T16-050588	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1800673/1	2
Caelo	SyrSpend [®] SF pH4 cherry aroma	1803724/2	1
Caelo	Water	18042901	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1806233/02	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1806233/2P-190927-3	1
Caelo	Water	18065601	3
Caelo	Water	18093501	3
Caelo	Water	18109501	1
Caelo	Water	18110401	4
Caelo	SyrSpend [®] SF pH4 aroma free	1812018	1
Caelo	Water	18156401	1
Caelo	Water	18178302	4
Caelo	Water	18178401	1
Caelo	Water	18226901	1
Caelo	Water	18228801	2
Caelo	Water	18238601	1
Caelo	Water	18254801	1
Caelo	Water	18263401	1
Caelo	Water	18265001	2
Caelo	Water	18305101	1
Caelo	Water	18305201	2
Caelo	Water	18305301	1
Caelo	Water	18305401	1
Caelo	Water	18325001	1
Caelo	Water	18E07-T08-055699	1
Caelo	Water	18E25-T01-056423	1
Caelo	Water	18G16-T05-058132	1
Caelo	Water	18J10-01-060845	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1900093P-190927-2	1
Caelo	SyrSpend [®] SF pH4 aroma free	19011410	2
Caelo	Water	19037701	1
Caelo	SyrSpend [®] SF pH4 aroma free	19061126	1

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Supplier	Substance	Batch	Spectra
Caelo	SyrSpend [®] SF pH4 aroma free	1906126	2
Caelo	Aloe vera gel, 10x concen...	19066601	2
Caelo	SyrSpend [®] SF pH4 cherry aroma	1909673	2
Caelo	Water	19152801	2
Caelo	Water	19184102	1
Caelo	Water	19184201	1
Caelo	Aloe vera gel, 10x concen...	19241101	1
Caelo	Water	19246201	1
Caelo	Aloe vera gel, 10x concen...	19255203	1
Caelo	Water	20000526002	1
Caelo	Water	20001119001	1
Caelo	Water	20002379002	1
Caelo	Water	20002911001	4
Caelo	Water	20003877001	6
Caelo	Water	20004435001	8
Caelo	SyrSpend [®] SF pH4 cherry aroma	20007312	2
Caelo	Water	21001086001	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	21002532	2
Caelo	Water	21003422001	1
Caelo	Water	21003609001	1
Caelo	Water	219181	1
Caelo	Water	22000150001	1
Caelo	Water	22002392001	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	22D11-T17-095910	1
Caelo	Water	LOTAP-SP0001	1
Caelo	Water	LOTAP0041	1
Caelo	Water	LOTAP0078	1
Caesar & Loretz GmbH...	Water	16127901	1
Caesar & Loretz GmbH	Aloe vera gel, 10x concen...	18125504	1
Caesar & Loretz GmbH	SyrSpend [®] SF pH4 cherry aroma	19000779004	1
Caesar & Loretz GmbH	Aloe vera gel, 10x concen...	192411002	1
Caesar & Loretz GmbH	Aloe vera gel, 10x concen...	19241101	1
Caesar & Loretz GmbH	Aloe vera gel, 10x concen...	20001962002	1
Caesar & Loretz GmbH	Water	20004264001	1
Caesar & Loretz GmbH	SyrSpend [®] SF pH4 aroma free	20009273	1
Caesar & Loretz GmbH	SyrSpend [®] SF pH4 cherry aroma	21000431001	1
Caesar & Loretz GmbH	SyrSpend [®] SF pH4 cherry aroma	21001852006	1
Caesar & Loretz GmbH	Water	22000953001	1
Caesar & Loretz GmbH	Water	22003907001	1
Caesar & Loretz GmbH...	Water	22001338001	2
Caesar & Loretz GmbH...	Water	22003129001	2
Caesar & Loretz/Noweda	Water	15394501	1
Chemica GmbH/ Rewe	Water	12345678	1
Dr.Wolff	Water	18061901	1
Eigen	Water	RD200626-0001	1
Eigenherstellung/Defektur	Water	5119E-01138	1
Euro OTC	Water	15F24-T01-023879	1
Euro OTC	Water	16F14-T07-034326	1
Euro OTC	SyrSpend [®] SF pH4 cherry aroma	1704492/01	1
Euro OTC	SyrSpend [®] SF pH4 cherry aroma	1900093	1
F/sa	Water	RM31/F24	1
Fagron	SyrSpend [®] SF pH4 aroma free		5
Fagron	SyrSpend [®] SF pH4 aroma free	102653/1	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	13359004	1
Fagron	SyrSpend [®] SF pH4 aroma free	1410D020	8
Fagron	SyrSpend [®] SF pH4 aroma free	1412D002	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	1503255	19
Fagron	SyrSpend [®] SF pH4 aroma free	1503D009	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	1503D017	2

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Supplier	Substance	Batch	Spectra
Fagron	SyrSpend [®] SF pH4 cherry aroma	1507318	5
Fagron	SyrSpend [®] SF pH4 aroma free	15C12/E	1
Fagron	SyrSpend [®] SF pH4 aroma free	15C12E	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	15C19/C	7
Fagron	Water	15D13-T07-021465	1
Fagron	Water	15D13-T09-021469	1
Fagron	Water	15H25-T14-025670	1
Fagron	Water	15H25-T18-025678	1
Fagron	Water	15H25-T21-025683	1
Fagron	Water	15K10-T04-027614	1
Fagron	Water	15K10-T08-027626	1
Fagron	Water	15L14-T14-028664	1
Fagron	Water	15L15-T01-028672	1
Fagron	Water	15L15-T07-028685	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1603252/2	12
Fagron	SyrSpend [®] SF pH4 aroma free	1609686	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1612631	22
Fagron	Water	16B10-T02-030206	1
Fagron	Water	16C22-T07-031410	1
Fagron	Water	16C22-T09-031414	1
Fagron	Water	16C23-T06-031423	1
Fagron	Water	16F13-T16-034297	2
Fagron	Water	16F13-T18-034301	1
Fagron	Water	16F14-T03-034317	1
Fagron	Water	16F14-T09-034330	1
Fagron	Water	16K25-C20-17409	1
Fagron	Water	16L12-T11-039624	1
Fagron	Water	16L12-T16-039628	1
Fagron	Water	16L12-T25-039642	2
Fagron	Aloe vera gel, 10x concen. ...	1701-5623	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1701543/3	5
Fagron	SyrSpend [®] SF pH4 cherry aroma	1702015	24
Fagron	SyrSpend [®] SF pH4 cherry aroma	1702015(2Flaschen)	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1704492/1	10
Fagron	SyrSpend [®] SF pH4 aroma free	1704493	11
Fagron	SyrSpend [®] SF pH4 cherry aroma	1704992/1	1
Fagron	SyrSpend [®] SF pH4 aroma free	1706769	1
Fagron	SyrSpend [®] SF pH4 aroma free	1706769/1	7
Fagron	SyrSpend [®] SF pH4 cherry aroma	1707032/1	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1707302/1	7
Fagron	SyrSpend [®] SF pH4 cherry aroma	1712017	6
Fagron	SyrSpend [®] SF pH4 aroma free	1712018	8
Fagron	SyrSpend [®] SF pH4 aroma free	1712023/02	1
Fagron	SyrSpend [®] SF pH4 aroma free	1712023/1	9
Fagron	SyrSpend [®] SF pH4 aroma free	1712023/2	30
Fagron	SyrSpend [®] SF pH4 cherry aroma	1712024	21
Fagron	SyrSpend [®] SF pH4 aroma free	17122018	1
Fagron	SyrSpend [®] SF pH4 aroma free	17202371	1
Fagron	Water	17B10-T20-041571	1
Fagron	Water	17B10-T27-041575	1
Fagron	Water	17C31-T05-043064	1
Fagron	Water	17E05-T01-044045	2
Fagron	Water	17E05-T03-044051	1
Fagron	Water	17E05-T05-044063	2
Fagron	Water	17E05-T13-044080	1
Fagron	Water	17E05T07044067	1
Fagron	Water	17E05T11044076	1
Fagron	Water	17F23-T06-045760	1

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Supplier	Substance	Batch	Spectra
Fagron	Water	17H24-T09-047709	1
Fagron	Water	17H24-T11-047713	1
Fagron	Water	17H24-T13-047717	1
Fagron	Water	17K27-T09-050544	2
Fagron	Water	17K27-T11-050552	4
Fagron	Water	17K27-T15-050585	2
Fagron	Water	17K27-T16-050588	1
Fagron	Water	17L20-T02-051255	1
Fagron	Water	17L20-T20-0001	1
Fagron	SyrSpend® SF pH4 cherry aroma	18000673/1	1
Fagron	SyrSpend® SF pH4 cherry aroma	180067/1	1
Fagron	SyrSpend® SF pH4 cherry aroma	1800673	1
Fagron	SyrSpend® SF pH4 cherry aroma	1800673/1	21
Fagron	SyrSpend® SF pH4 cherry aroma	1800673/1P-180827-1	1
Fagron	SyrSpend® SF pH4 cherry aroma	1800673/2	1
Fagron	SyrSpend® SF pH4 aroma free	18025653/1	1
Fagron	SyrSpend® SF pH4 aroma free	1802653/1	21
Fagron	SyrSpend® SF pH4 aroma free	1802653/2	5
Fagron	SyrSpend® SF pH4 aroma free	1802653/4	2
Fagron	SyrSpend® SF pH4 aroma free	18026531	1
Fagron	SyrSpend® SF pH4 aroma free	1802654	9
Fagron	SyrSpend® SF pH4 cherry aroma	1802928	6
Fagron	SyrSpend® SF pH4 cherry aroma	1803724/2	36
Fagron	SyrSpend® SF pH4 cherry aroma	1803724/2P-180922-1	1
Fagron	SyrSpend® SF pH4 aroma free	1804245-2	1
Fagron	SyrSpend® SF pH4 aroma free	1804245/1	25
Fagron	SyrSpend® SF pH4 aroma free	1804245/2	2
Fagron	SyrSpend® SF pH4 aroma free	18042451	1
Fagron	SyrSpend® SF pH4 cherry aroma	1806233/1	5
Fagron	SyrSpend® SF pH4 cherry aroma	1806233/2	38
Fagron	SyrSpend® SF pH4 cherry aroma	1806233/2P-190618-2	1
Fagron	SyrSpend® SF pH4 cherry aroma	1806233/2P-190808-3	1
Fagron	SyrSpend® SF pH4 cherry aroma	18062331	1
Fagron	SyrSpend® SF pH4 cherry aroma	180623312	1
Fagron	SyrSpend® SF pH4 aroma free	1808206-2	1
Fagron	SyrSpend® SF pH4 aroma free	1808206/1	3
Fagron	SyrSpend® SF pH4 aroma free	1808206/12	1
Fagron	SyrSpend® SF pH4 aroma free	1808206/2	62
Fagron	SyrSpend® SF pH4 aroma free	1808206/2A	1
Fagron	SyrSpend® SF pH4 aroma free	1808206/2B	1
Fagron	SyrSpend® SF pH4 aroma free	18082062	1
Fagron	SyrSpend® SF pH4 aroma free	1812150/2	16
Fagron	SyrSpend® SF pH4 aroma free	1814231	31
Fagron	SyrSpend® SF pH4 cherry aroma	1860233/2	1
Fagron	Water	18c13-T14-053737	1
Fagron	Water	18C19-T25	1
Fagron	Water	18C19-T28-054003	1
Fagron	Water	18C19-T29-054007	2
Fagron	Water	18C19-T30-054012	2
Fagron	Water	18C19-T31-054017	2
Fagron	Water	18C19T31054017	1
Fagron	SyrSpend® SF pH4 aroma free	18c2653/1	1
Fagron	Water	18E07-T08-055699	1
Fagron	Water	18E09-T0-055711	1
Fagron	Water	18E25-T01-056423	2
Fagron	Water	18E28-T02-056492	1
Fagron	Water	18G16-T01-058118	1
Fagron	Water	18G16-T02-058123	1

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Supplier	Substance	Batch	Spectra
Fagron	Water	18G16-T04-058129	2
Fagron	Water	18G16-T05-058132	1
Fagron	Water	18L19To6o62853	1
Fagron	SyrSpend® SF pH4 cherry aroma	1900093	28
Fagron	SyrSpend® SF pH4 cherry aroma	19009673	1
Fagron	SyrSpend® SF pH4 aroma free	19011210	1
Fagron	SyrSpend® SF pH4 aroma free	19011410	87
Fagron	SyrSpend® SF pH4 aroma free	190114110	1
Fagron	SyrSpend® SF pH4 cherry aroma	1904383	1
Fagron	SyrSpend® SF pH4 aroma free	1906126	38
Fagron	SyrSpend® SF pH4 aroma free	1907122	29
Fagron	SyrSpend® SF pH4 cherry aroma	1908041	1
Fagron	SyrSpend® SF pH4 cherry aroma	19094223/2	1
Fagron	SyrSpend® SF pH4 cherry aroma	1909423-2	1
Fagron	SyrSpend® SF pH4 cherry aroma	1909423/1	18
Fagron	SyrSpend® SF pH4 cherry aroma	1909423/2	5
Fagron	SyrSpend® SF pH4 cherry aroma	19094231	1
Fagron	SyrSpend® SF pH4 cherry aroma	1909673	58
Fagron	SyrSpend® SF pH4 cherry aroma	190973	1
Fagron	SyrSpend® SF pH4 aroma free	1911010	6
Fagron	SyrSpend® SF pH4 aroma free	19911010	1
Fagron	Water	19A18-T07-063531	3
Fagron	Water	19A18-T08-063538	1
Fagron	Water	19E20-T09-067577	1
Fagron	Water	19H12-T16-070787	1
Fagron	Water	19h4-T09-072696	1
Fagron	Water	19h4-T10-072699	1
Fagron	Water	19h4-T12-072715	6
Fagron	Water	19J14-T07-072690	1
Fagron	Water	19J14-T08_072693	1
Fagron	SyrSpend® SF pH4 cherry aroma	200000326	2
Fagron	SyrSpend® SF pH4 cherry aroma	20000326	90
Fagron	SyrSpend® SF pH4 cherry aroma	20000326P-200709-3	1
Fagron	SyrSpend® SF pH4 cherry aroma	200007312	3
Fagron	SyrSpend® SF pH4 cherry aroma	2000326	3
Fagron	SyrSpend® SF pH4 aroma free	20004219	58
Fagron	SyrSpend® SF pH4 aroma free	20004220	18
Fagron	SyrSpend® SF pH4 cherry aroma	20004221	14
Fagron	SyrSpend® SF pH4 cherry aroma	20004332	50
Fagron	SyrSpend® SF pH4 cherry aroma	20004369	3
Fagron	SyrSpend® SF pH4 cherry aroma	200047312	1
Fagron	SyrSpend® SF pH4 aroma free	20006608	53
Fagron	SyrSpend® SF pH4 cherry aroma	20006936	20
Fagron	SyrSpend® SF pH4 cherry aroma	20007125	48
Fagron	SyrSpend® SF pH4 cherry aroma	20007130	10
Fagron	SyrSpend® SF pH4 cherry aroma	20007312	70
Fagron	SyrSpend® SF pH4 cherry aroma	20007312mfa	1
Fagron	SyrSpend® SF pH4 cherry aroma	20007317	21
Fagron	SyrSpend® SF pH4 aroma free	20007561	1
Fagron	SyrSpend® SF pH4 aroma free	20007563	26
Fagron	SyrSpend® SF pH4 aroma free	20007575	16
Fagron	SyrSpend® SF pH4 aroma free	20009273	67
Fagron	SyrSpend® SF pH4 cherry aroma	2006936	1
Fagron	SyrSpend® SF pH4 cherry aroma	2007312	2
Fagron	SyrSpend® SF pH4 aroma free	2009273	2
Fagron	Water	20C31-T19-078892	32
Fagron	Water	20D06-T17-078573	1

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Supplier	Substance	Batch	Spectra
Fagron	Water	20D08-T06-078666	4
Fagron	Water	20D14-725-078895	1
Fagron	Water	20D14-T25-078895	14
Fagron	Water	20G14-T-06-081572	1
Fagron	Water	20G14-T08-081578	6
Fagron	Water	20L22-T02-085064	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	21002532	57
Fagron	SyrSpend [®] SF pH4 aroma free	21005761	10
Fagron	SyrSpend [®] SF pH4 cherry aroma	21008809	4
Fagron	SyrSpend [®] SF pH4 aroma free	21009136	38
Fagron	SyrSpend [®] SF pH4 aroma free	21009136/2301251	1
Fagron	SyrSpend [®] SF pH4 aroma free	21009236	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	21010483	53
Fagron	SyrSpend [®] SF pH4 cherry aroma	21020483	1
Fagron	Water	21D19-T10-087703	2
Fagron	Water	21G28-T25-090471	1
Fagron	SyrSpend [®] SF pH4 aroma free	22000887	16
Fagron	SyrSpend [®] SF pH4 aroma free	22092007	1
Fagron	SyrSpend [®] SF pH4 aroma free	22092008	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	22B24-T01	1
Fagron	SyrSpend [®] SF pH4 aroma free	22D11-T08	5
Fagron	SyrSpend [®] SF pH4 aroma free	22d11-t08-095894	1
Fagron	SyrSpend [®] SF pH4 aroma free	22D11-T08-095894	2
Fagron	SyrSpend [®] SF pH4 aroma free	22D11-T09	4
Fagron	SyrSpend [®] SF pH4 aroma free	22d11-t09-095898	1
Fagron	SyrSpend [®] SF pH4 aroma free	22D11-T09-095898	27
Fagron	SyrSpend [®] SF pH4 aroma free	22D11-T09-095899	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11-T17-095910	17
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11-T17-095911	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11-T18	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11-T18-05918	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11-T18-095918	8
Fagron	SyrSpend [®] SF pH4 aroma free	22D11T05095898	1
Fagron	SyrSpend [®] SF pH4 aroma free	22D11T09	1
Fagron	SyrSpend [®] SF pH4 aroma free	22D11T09095898	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11T17095910	1
Fagron	Water	22E27-T13	1
Fagron	SyrSpend [®] SF pH4 aroma free	22H11-165220	1
Fagron	SyrSpend [®] SF pH4 aroma free	22H11-T09	2
Fagron	SyrSpend [®] SF pH4 aroma free	22H11-T09-099022	16
Fagron	SyrSpend [®] SF pH4 aroma free	22H11-T10-099025	8
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T11-099029	6
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T11-099030	5
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T13	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T13-099034	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T13-099035	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T17-095910	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T18	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T18-099038	26
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-TT18-099038	1
Fagron	SyrSpend [®] SF pH4 aroma free	22H11T10099025	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H13-099035	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H30-T05-099074	4
Fagron	SyrSpend [®] SF pH4 aroma free	22H30-T05-099074	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22I14-T22	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22J14-T08	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	22j14-t08-100064	3

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Supplier	Substance	Batch	Spectra
Fagron	SyrSpend [®] SF pH4 cherry aroma	22J14-T08-100064	8
Fagron	SyrSpend [®] SF pH4 cherry aroma	22J14-T08-100065	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	22J14-T08	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22J14-T08-100065	1
Fagron	SyrSpend [®] SF pH4 aroma free	23809-T05-102908	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	23A05-T07-102866	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	23A10-T20-102143	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	23A26-T03-102457	11
Fagron	SyrSpend [®] SF pH4 cherry aroma	23A26-T03	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	23A05-T07-102866	1
Fagron	SyrSpend [®] SF pH4 aroma free	23B09-t05	1
Fagron	SyrSpend [®] SF pH4 aroma free	23B09-T05-102908	6
Fagron	SyrSpend [®] SF pH4 aroma free	23B10-T02-102920	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	23B17-T02-103078	1
Fagron	SyrSpend [®] SF pH4 aroma free	23B17-T03-103124	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	23E12-T02-105247	1
Fagron	SyrSpend [®] SF pH4 aroma free	23E19-716-105390	1
Fagron	SyrSpend [®] SF pH4 aroma free	23E19-T12	1
Fagron	SyrSpend [®] SF pH4 aroma free	27121704	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	2x1712024	1
Fagron	SyrSpend [®] SF pH4 aroma free	3103124	1
Fagron	SyrSpend [®] SF pH4 aroma free	4415A-07040	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	4415A-07041	1
Fagron	SyrSpend [®] SF pH4 aroma free	518E-07040	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	518E-07041	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	720023-0003	5
Fagron	SyrSpend [®] SF pH4 aroma free	720024-0003	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	A05-T07-1028606	1
Fagron	Water	T07-0872009	1
Fagron	SyrSpend [®] SF pH4 aroma free	T09-0958908	1
Fagron	SyrSpend [®] SF pH4 aroma free	T09-0958909	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	T13-0990305	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	T17-095910	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	T17-0959100	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	T18-0959108	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	T20-1021403	1
Fagron	SyrSpend [®] SF pH4 aroma free	T08-0958904	1
Fagron	SyrSpend [®] SF pH4 aroma free	T09-0958908	1
Fargon	SyrSpend [®] SF pH4 cherry aroma	1900093	1
Fargon	SyrSpend [®] SF pH4 cherry aroma	1909673	2
Fargon/AHD	SyrSpend [®] SF pH4 cherry aroma	1806233/2	1
Fargon/Gehe	Water	19A18-T07-063531	1
Fargon/Gehe	SyrSpend [®] SF pH4 cherry aroma	20007312	2
Fargon/Gehe	SyrSpend [®] SF pH4 cherry aroma	20007317	1
Fargon/Kehr	Water	16F13-T18-034301	1
Fargon / GEHE	SyrSpend [®] SF pH4 cherry aroma	1900093	1
Fargon/Phönix	Water	18C19-T31-054017	1
Fargon/PNACH	SyrSpend [®] SF pH4 aroma free	1712023/1	1
Fgron / Kehr 03.02.2020	SyrSpend [®] SF pH4 aroma free	1812150/2	1
Fgron	SyrSpend [®] SF pH4 aroma free	22000887	1
Fiebig	SyrSpend [®] SF pH4 cherry aroma	20000326	1
Fiebig	SyrSpend [®] SF pH4 cherry aroma	20004221	2
Fiebig	SyrSpend [®] SF pH4 cherry aroma	20004332	2
Fiebig	SyrSpend [®] SF pH4 cherry aroma	20006936	1
Fiebig	SyrSpend [®] SF pH4 cherry aroma	20007312	1
Fiebig	SyrSpend [®] SF pH4 cherry aroma	20007317	1
Fiebig/Fagon	SyrSpend [®] SF pH4 cherry aroma	20004332	1

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Supplier	Substance	Batch	Spectra
Fragron	SyrSpend [®] SF pH4 cherry aroma	1702015	1
Fresenius /Noweda	Water	19KK24GA	1
Fresenius	Water	19LM27GA	1
GEHE	Water	17114801	1
Gehe	SyrSpend [®] SF pH4 aroma free	1712023/1	4
GEHE	SyrSpend [®] SF pH4 cherry aroma	1712024	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	17122017	1
Gehe	Water	17219101	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	1803724/2	1
GEHE	SyrSpend [®] SF pH4 cherry aroma	1803724/2	3
GEHE	SyrSpend [®] SF pH4 cherry aroma	1806233/2	2
Gehe	SyrSpend [®] SF pH4 aroma free	1808206/2	7
Gehe	SyrSpend [®] SF pH4 aroma free	1812150/2	2
Gehe	SyrSpend [®] SF pH4 aroma free	1814231	3
Gehe	SyrSpend [®] SF pH4 aroma free	19011410	6
Gehe	SyrSpend [®] SF pH4 aroma free	1906126	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	1909423/1	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	1909673	1
Gehe	SyrSpend [®] SF pH4 aroma free	1911010	1
Gehe	SyrSpend [®] SF pH4 aroma free	20004219	2
Gehe	SyrSpend [®] SF pH4 aroma free	20006608	4
Gehe	SyrSpend [®] SF pH4 cherry aroma	20007152	1
Gehe	SyrSpend [®] SF pH4 aroma free	20009273	1
GEHE	SyrSpend [®] SF pH4 aroma free	20009273	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	21002532	2
GEHE	SyrSpend [®] SF pH4 cherry aroma	21002532	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	21010483	1
Gehe	Water	22003905002	1
GEHE	SyrSpend [®] SF pH4 cherry aroma	22H11-T18-099038	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	23A05-T07-102866	2
Gehe	SyrSpend [®] SF pH4 aroma free	23A24-T16-106100	2
gehe	SyrSpend [®] SF pH4 cherry aroma	23a26-T05-102460	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	23A26-T03-102457	1
Gehe	SyrSpend [®] SF pH4 aroma free	23B09-T05-102908	3
Gehe	SyrSpend [®] SF pH4 cherry aroma	23B17-T02	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	23B17-T02-103078	2
Gehe	SyrSpend [®] SF pH4 cherry aroma	23C08-T03	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	23C13_T07	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	23C13-T07	1
Gehe	SyrSpend [®] SF pH4 aroma free	23E19-T15-105387	3
Gehe	SyrSpend [®] SF pH4 aroma free	23E19-T16-105390	3
Gehe	SyrSpend [®] SF pH4 cherry aroma	23E22-T04-105414	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	23E22T05-105417	1
Gehe	Water	T10-0970904	1
GMP konforme	SyrSpend [®] SF pH4 cherry aroma	21010483	1
GUMO	SyrSpend [®] SF pH4 aroma free	19011410	1
GUMO	SyrSpend [®] SF pH4 cherry aroma	20000326	1
GUMO	SyrSpend [®] SF pH4 cherry aroma	20004221	1
GUMO	SyrSpend [®] SF pH4 cherry aroma	20007312	1
Hedinger	Water	219140	1
HEDINGER	Water	219162	1
Hedinger	Water	219208	1
HEDINGER	Water	LOTAP0071	1
Hedinger/Noweda	Water	219209	6
Hedinger/Noweda	Water	219212	9
Hedinger/Phoenix	Water	219206	4
Hedinger/Phoenix	Water	219222	6

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Supplier	Substance	Batch	Spectra
Hedinger/Phoenix	Water	219227	1
Henry Lamotte Oil / Gehe	Water	17K27-T10-050547	1
Herkel B.V. / AHD	SyrSpend® SF pH4 cherry aroma	21002532	4
Herkel B.V./Kehr	SyrSpend® SF pH4 aroma free	1808206/2	1
Herkel B.V./Phönix	SyrSpend® SF pH4 cherry aroma	20007312	1
Holdermann	SyrSpend® SF pH4 aroma free	23B02-T16-106339	1
Ichthyol/Gehe	SyrSpend® SF pH4 cherry aroma	1900093	1
Jenne	SyrSpend® SF pH4 cherry aroma	1900093	2
Kehr	SyrSpend® SF pH4 cherry aroma	22H11-T13-099034	2
kehr	SyrSpend® SF pH4 aroma free	22H11T09099022	1
kehr	SyrSpend® SF pH4 cherry aroma	22H11T11099029	1
Kehr	SyrSpend® SF pH4 cherry aroma	22I14-T22-099449	3
Kehr	SyrSpend® SF pH4 cherry aroma	22I14-T22-099449	1
Kehr	SyrSpend® SF pH4 cherry aroma	23A05-T07-102866	2
Kehr	SyrSpend® SF pH4 cherry aroma	23A10-T20-102143	1
kehr	SyrSpend® SF pH4 aroma free	23b02t16106339	1
Kehr	SyrSpend® SF pH4 aroma free	23D05-T03-104272	2
Kehr.21.07.2020	SyrSpend® SF pH4 cherry aroma	20000326	1
Kehr.26.03.2020	SyrSpend® SF pH4 aroma free	1814231	1
kerndl-Noweda	Water		2
Krieger	SyrSpend® SF pH4 aroma free	20004219	2
Krieger	SyrSpend® SF pH4 aroma free	23B17-T03-103124	1
L30	Water	17291301	1
Midas	Water	16C22-T07-031410	1
Midas	Water	16L12-T25-039642	1
Midas	Water	21001409001	1
Neue Adler Apotheke SFT	Water	23/12/2021	1
Noveda	Water	24A11-T06-110740	1
noweda	SyrSpend® SF pH4 cherry aroma	1612631	1
Noweda	SyrSpend® SF pH4 cherry aroma	1702015	1
Noweda	SyrSpend® SF pH4 aroma free	1712023/2	3
Noweda	Water	17E05-T03-044051	1
Noweda	SyrSpend® SF pH4 cherry aroma	1800673/1	1
Noweda	SyrSpend® SF pH4 aroma free	1804245/2	1
Noweda	SyrSpend® SF pH4 aroma free	1808206/2	1
Noweda	SyrSpend® SF pH4 cherry aroma	1909673	1
Noweda	SyrSpend® SF pH4 aroma free	20004220	1
Noweda	SyrSpend® SF pH4 aroma free	2006608	1
Noweda	SyrSpend® SF pH4 cherry aroma	21002532	1
Noweda	SyrSpend® SF pH4 aroma free	21009136	2
Noweda	SyrSpend® SF pH4 cherry aroma	21010483	2
Noweda	SyrSpend® SF pH4 cherry aroma	22/14-T08-100064	2
noweda	SyrSpend® SF pH4 cherry aroma	22114-T22-099449	1
noweda	SyrSpend® SF pH4 aroma free	22D11-T09-095898	1
Noweda	SyrSpend® SF pH4 aroma free	22D11-T09-095898	2
Noweda	SyrSpend® SF pH4 aroma free	22D11T09095898/2305020	1
Noweda	SyrSpend® SF pH4 aroma free	22H11-T09-099022	2
Noweda	SyrSpend® SF pH4 cherry aroma	23C13-T07-103723	1
Noweda	SyrSpend® SF pH4 cherry aroma	23E12-T02-105247	1
Noweda	SyrSpend® SF pH4 cherry aroma	23E12-T02-105247	1
Noweda	SyrSpend® SF pH4 aroma free	23E19-T12	3
Noweda	Water	436461	1
Otto Fischar	Water	90459/1	1
Phoenixx	SyrSpend® SF pH4 aroma free	23B17-T03-103124	1
Phoenix	SyrSpend® SF pH4 cherry aroma	15C19/C	1
Phoenix	Water	15L14-T14-028664	1
Phoenix	SyrSpend® SF pH4 cherry aroma	1603252/2	1

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Supplier	Substance	Batch	Spectra
Phoenix	SyrSpend® SF pH4 aroma free	1804245/1	8
Phoenix	SyrSpend® SF pH4 aroma free	19011410	2
Phoenix	SyrSpend® SF pH4 cherry aroma	1909423/1	1
Phoenix	SyrSpend® SF pH4 cherry aroma	20000326	1
Phoenix	Water	20003877001	1
Phoenix	SyrSpend® SF pH4 aroma free	20004220	1
Phoenix	SyrSpend® SF pH4 cherry aroma	20004332	2
Phoenix	SyrSpend® SF pH4 aroma free	200069608	1
Phoenix	SyrSpend® SF pH4 cherry aroma	23A26-T03-102457	1
Phoenix	Water	3387	1
Phoenix	SyrSpend® SF pH4 aroma free	720024-0003	1
Phönix EK:8,37 EUR 2L	Water	17B10-T18-041564	1
Phönix Gotha	SyrSpend® SF pH4 aroma free	1802653/1	2
Phönix Gotha	SyrSpend® SF pH4 aroma free	1802654	4
Phönix Gotha	SyrSpend® SF pH4 cherry aroma	1909673	1
Phönix Gotha	SyrSpend® SF pH4 cherry aroma	20000326	2
Phönix, Caesar&Loret...	SyrSpend® SF pH4 cherry aroma	20004332	1
Phönix	SyrSpend® SF pH4 cherry aroma		2
PHÖNIX	SyrSpend® SF pH4 cherry aroma	1704492/1	1
Phönix	SyrSpend® SF pH4 aroma free	1802653/01	1
Phönix	SyrSpend® SF pH4 aroma free	1802653/1	1
Phönix	Water	18C19-T25-053991	1
Phönix	SyrSpend® SF pH4 cherry aroma	1909673	2
Phönix	SyrSpend® SF pH4 cherry aroma	20004332	4
Phönix	SyrSpend® SF pH4 aroma free	20006608	1
Phönix	SyrSpend® SF pH4 cherry aroma	20007125	2
Phönix	SyrSpend® SF pH4 cherry aroma	20007130	1
Phönix	SyrSpend® SF pH4 aroma free	20009273	2
PHönix	SyrSpend® SF pH4 cherry aroma	21002532	1
Phönix	SyrSpend® SF pH4 cherry aroma	22D11-T17	1
Phönix	SyrSpend® SF pH4 aroma free	23810-T02-102920	1
Phönix	SyrSpend® SF pH4 aroma free	23B10-T02-102920	1
Phönix	SyrSpend® SF pH4 aroma free	23B17-T03-103124	3
Phönix	SyrSpend® SF pH4 aroma free	23E19-T12-105376	2
Phönix	SyrSpend® SF pH4 aroma free	23E19-T15-105387	1
phönix	SyrSpend® SF pH4 aroma free	23E19-T16-105390	1
Phönix	SyrSpend® SF pH4 cherry aroma	23E22-T05-105417	3
Phönix	SyrSpend® SF pH4 cherry aroma	23E22-T15-105455	1
Phönix	Water	23K06-T07-108661	1
Phönix	Water	LOTAP0154	1
Phönix/Fagro GmbH&Co...	SyrSpend® SF pH4 aroma free	20004219	1
Resana/Phönix	Aloe vera gel, 10x concen...	1901-6285	1
Retterspitz/ Phoenix	Retterspitz external	17224	1
Retterspitz/ Phoenix	Retterspitz external	18045	1
S/M	Water	906754	1
S/M	Water	RM31/24	1
S/M	Water	RM31/3	1
Sanacorp	SyrSpend® SF pH4 cherry aroma	1712017	2
Sanacorp	Water	18042901	1
Sanacorp	SyrSpend® SF pH4 aroma free	19011410	1
Sanacorp	SyrSpend® SF pH4 cherry aroma	1909673	2
Sanacorp	SyrSpend® SF pH4 aroma free	20004219	2
Sanacorp	SyrSpend® SF pH4 cherry aroma	20007130	1
Sanacorp	SyrSpend® SF pH4 aroma free	20009273	4
Sanacorp	SyrSpend® SF pH4 aroma free	22000887	1
Sanacorp	SyrSpend® SF pH4 cherry aroma	22D11-T17-095910	1
Sanacorp	SyrSpend® SF pH4 cherry aroma	22H11-T11-099029	1

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Supplier	Substance	Batch	Spectra
Sanacorp	SyrSpend [®] SF pH4 cherry aroma	22H11-T13-099034	1
Sanacorp	SyrSpend [®] SF pH4 aroma free	23b10-t02-102920	1
Sanacorp	SyrSpend [®] SF pH4 aroma free	23B10-T02-102920	2
Sanacorp/Wepa	Water	LOTAP-SP0003	1
serumwerk bernburg - Gehe	Water		5
Serumwerk Bernburg AG	Water		1
Serumwerk Bernburg	Water		1
Sonne Defektur	Water	422I-01138	1
Sonne Defektur	Water	5122Q-01138	1
Spinnrad	Aloe vera gel, 10x concen...	319502021	1
Tiofarma B.V.	SyrSpend [®] SF pH4 aroma free	1410D020	1
Walter Schmidt Chemi...	Water	95058	1
Wepa / Sanacorp	Water	LotAP0088	1
WEPA Apothekenbedarf...	Water	LOTAP0158	1
WEPA Apothekenbedarf...	Water	LOTAP0095	1
Wepa Apothekenbedarf	Water	LOTAP0050	1
Wepa Phönix	Water	LOTAPSP0003	1
wepa	Water	AP00036	1
Wepa	Water	AP0072	1
Wepa	Water	LOTAP-SP0001	1
Wepa	Water	LOTAP-SP0002	1
Wepa	Water	LOTAP-SP0004	1
WEPA	Water	LOTAP-SP0005	1
Wepa	Water	LOTAP-SP0006	1
Wepa	Water	LOTAP-SP0010	1
WEPA	Water	LOTAP-SP0027	1
WEPA	Water	LOTAP0015	1
wepa	Water	LOTAP0019	1
Wepa	Water	LOTAP0020	1
Wepa	Water	LOTAP0031	1
wepa	Water	LOTAP0034	1
WEPA	Water	LOTAP0068	1
Wepa	Water	LOTAP0072	1
wepa	Water	LOTAP0075	1
Wepa	Water	LOTAP0080	1
WEPA	Water	LOTAP0081	1
Wepa	Water	LOTAP0084	1
Wepa	Water	LOTAP0087	1
Wepa	Water	LOTAP0123	1
Wepa	Water	LOTAP0144	1
Wepa/ Wepa	Water	LOTAP0077	1
Wepa/AHCA	Water	LOTAP0099	1
WEPA/Krieger	Water	LOTAP0086	1
Wepa/Wepa	Water	LOTAP-SP0023	1
Wepa/Wepa	Water	LOTAP0037	1
WEPA/WEPA	Water	LOTAP0088	1
Wepa/Wepa	Water	LOTAP0112	1
Wepa/Wepa/ 13.05.201...	Water	LOTAP0101	1

- 17 655 spectra from 1481 *Apo-Ident* customers from a total of 5719 batches from a further 162 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Water and aqueous solutions* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Water and aqueous solutions* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	1005	0	26 929
Type B	0	2795	10	27 005
Type C	0	3108	15	17 591

The substance/substance group *Water and aqueous solutions* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9613 %)	100.0000 % (> 99.4030 %)
Type B	100.0000 % (> 99.9563 %)	99.6435 % (> 99.5365 %)
Type C	100.0000 % (> 99.0540 %)	99.5197 % (> 99.4236 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31146	31146	0.00	28.24
31623	31623	0.00	30.08
31670	31670	0.00	29.02
31671	31671	0.00	29.63
31675	31675	0.00	32.24
31722	31722	0.00	28.49
31723	31723	0.00	28.60
31862	31862	0.00	27.93
32079	32079	0.00	30.85
32313	32313	0.00	27.54
32785	32785	0.00	23.11
33430	33430	0.00	25.86
33431	33431	0.00	25.63
33787	33787	0.00	27.93
34767	34767	0.00	31.01
35049	35049	0.00	24.06

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
35077	35077	0.00	27.43
35239	35239	0.00	30.49
35240	35240	0.00	30.23
35242	35242	0.00	30.11
36745	36745	0.00	27.88
38624	38624	0.00	28.76

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Wax ointment**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31111-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Wax ointment; Unguentum cereum

Special notes

When selecting the *Wax ointment* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Wax ointment	6	15	98

Second-stage model

For differentiation of the substance/substance group *Wax ointment* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Wax ointment* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cottonwood ointment	17.57	—
Protegin [®] XN	21.20	—
Marjoram ointment	21.43	—
Neribas [®] fat ointment	25.39	—
Balm Bio Nature	34.75	—
Deumavan [®] protection ointment neutral	36.98	—
White paraffin oil	40.16	—
Asche Basis [®] fat ointment	50.06	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Wax ointment* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Wax ointment*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Wax ointment	13072102	31111	40	not required
Caelo	Wax ointment	13307701	31167	40	not required
Caelo	Wax ointment	14073701	31444	40	not required
Caelo	Wax ointment	154243	31911	60	20151217*
Caelo	Wax ointment	154244	31912	60	20151217*
Caelo	Wax ointment	22001707	36402	40	20220705*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 6 reference samples from the substance/substance group *Wax ointment*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 6 different batches.
- 27 654 spectra from a total of 594 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 540 spectra of 15 reference samples from the substance/substance group *Wax ointment*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Wax ointment	12352501	30967	40
Caelo	Wax ointment	161215	32117	40
Caelo	Wax ointment	161334	32118	40
Caelo	Wax ointment	171714	33550	40
Caelo	Wax ointment	172942	34024	40
Caelo	Wax ointment	191905	34793	40
Caelo	Wax ointment	19000784	34984	40
Caelo	Wax ointment	20002322	35095	40
Caelo	Wax ointment	21003702	35985	40
Caelo	Wax ointment	22002672	36652	40
Caelo	Wax ointment	23000483	36971	40
Caelo	Wax ointment	23000484	36972	10
Caelo	Wax ointment	23002428	37824	40
Caelo	Wax ointment	24001166	38334	40
Caelo	Wax ointment	24001167	38335	10

- 30 390 spectra from a total of 694 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 869 spectra from 323 *Apo-Ident* customers from 102 batches from the substance/substance group *Wax ointment*.
- Among them are spectra of independent samples from 98 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Wax ointment	21002596001	1
	Wax ointment	21003702002	1
	Wax ointment	22002672001	6
	Wax ointment	22002672002	1
	Wax ointment	23000483001	23
	Wax ointment	23000484001	1
	Wax ointment	23002256001	1
	Wax ointment	23002428001	9
	Wax ointment	24001166001	5
AHD	Wax ointment	14073701	1
AHD	Wax ointment	24001166001	1
Alliance Healthcare	Wax ointment	18162202	1
Alliance Healthcare	Wax ointment	19190502	2
Anzag 07.12.12	Wax ointment	12128702	1
Caello/Phönix	Wax ointment	16121501	2
Caelo	Wax ointment		1
Caelo	Wax ointment	1000337003	1
Caelo	Wax ointment	1021303	1
Caelo	Wax ointment	1114E3212	1
Caelo	Wax ointment	11321302	1
Caelo	Wax ointment	11355201	2
Caelo	Wax ointment	11355202	1
Caelo	Wax ointment	12033602	2
Caelo	Wax ointment	12033701	4
Caelo	Wax ointment	1218702	2
Caelo	Wax ointment	12209401	3
Caelo	Wax ointment	12209402	1
Caelo	Wax ointment	12352051	1
Caelo	Wax ointment	12352501	4
Caelo	Wax ointment	12378701	5
Caelo	Wax ointment	13072102	13
Caelo	Wax ointment	13159302	7
Caelo	Wax ointment	13159303	2
Caelo	Wax ointment	13307701	17
Caelo	Wax ointment	13307802	13
Caelo	Wax ointment	14072801	1
Caelo	Wax ointment	1407301	1
Caelo	Wax ointment	14073701	15
Caelo	Wax ointment	140737012	1
Caelo	Wax ointment	140737701	1
Caelo	Wax ointment	14073801	7
Caelo	Wax ointment	14073802	1
Caelo	Wax ointment	14235901	13
Caelo	Wax ointment	14236001	3
Caelo	Wax ointment	14236002	4
Caelo	Wax ointment	14236003	1
Caelo	Wax ointment	15025701	1
Caelo	Wax ointment	15025702	11
Caelo	Wax ointment	15025801	17
Caelo	Wax ointment	15205402	13

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Supplier	Substance	Batch	Spectra
Caelo	Wax ointment	1524301	1
Caelo	Wax ointment	1524401	1
Caelo	Wax ointment	15424301	19
Caelo	Wax ointment	15424401	9
Caelo	Wax ointment	15424402	4
Caelo	Wax ointment	16121501	8
Caelo	Wax ointment	16121502	4
Caelo	Wax ointment	16133401	22
Caelo	Wax ointment	17014901	27
Caelo	Wax ointment	17015001	21
Caelo	Wax ointment	17015002	1
Caelo	Wax ointment	17171401	21
Caelo	Wax ointment	17294201	21
Caelo	Wax ointment	17294202	16
Caelo	Wax ointment	18034601	3
Caelo	Wax ointment	18034602	21
Caelo	Wax ointment	18162201	7
Caelo	Wax ointment	18162202	14
Caelo	Wax ointment	18258501	28
Caelo	Wax ointment	19000783001	35
Caelo	Wax ointment	19000784001	6
Caelo	Wax ointment	19000784002	12
Caelo	Wax ointment	19040001	10
Caelo	Wax ointment	19040002	23
Caelo	Wax ointment	19040003	5
Caelo	Wax ointment	19190501	30
Caelo	Wax ointment	19190502	3
Caelo	Wax ointment	200003013002	1
Caelo	Wax ointment	20002187004	1
Caelo	Wax ointment	20002322002	15
Caelo	Wax ointment	20003013001	8
Caelo	Wax ointment	20003013002	7
Caelo	Wax ointment	20051012-1	1
Caelo	Wax ointment	20121305	1
Caelo	Wax ointment	21000337001	3
Caelo	Wax ointment	21000337002	12
Caelo	Wax ointment	21000337003	1
Caelo	Wax ointment	21000337225	1
Caelo	Wax ointment	2100259002	1
Caelo	Wax ointment	21002596001	13
Caelo	Wax ointment	21002596002	2
Caelo	Wax ointment	21002596003	1
Caelo	Wax ointment	21003702001	3
Caelo	Wax ointment	21003702002	1
Caelo	Wax ointment	21003702003	6
Caelo	Wax ointment	2113Q-03212	1
Caelo	Wax ointment	22001707001	3
Caelo	Wax ointment	22001707003	1
Caelo	Wax ointment	22002672001	2
Caelo	Wax ointment	220204A	1
Caelo	Wax ointment	23000484001	1
Caelo	Wax ointment	270120-01	1
Caelo	Wax ointment	28051511	1
Caelo	Wax ointment	3427	1
Caelo	Wax ointment	7071204	1
Caelo	Wax ointment	9531609	1
Caelo	Wax ointment	U-150513-2	1
Caeol/Noweda	Wax ointment	17294201	1
Caeol/Phoenix	Wax ointment	15424301	1
Caesar & Loretz GmbH...	Wax ointment	21003702002	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Wax ointment	13072102	1
Caesar & Loretz GmbH	Wax ointment	18162202	2
Caesar & Loretz GmbH	Wax ointment	18258501	7
Caesar & Loretz GmbH	Wax ointment	19000783001	8
Caesar & Loretz GmbH	Wax ointment	19000784002	3
Caesar & Loretz GmbH	Wax ointment	19040001	4
Caesar & Loretz GmbH	Wax ointment	19040002	3
Caesar & Loretz GmbH	Wax ointment	19190501	11
Caesar & Loretz GmbH	Wax ointment	19190502	7
Caesar & Loretz GmbH	Wax ointment	20002322001	2
Caesar & Loretz GmbH	Wax ointment	20002322002	9
Caesar & Loretz GmbH	Wax ointment	20003013002	6
Caesar & Loretz GmbH	Wax ointment	21000337001	2
Caesar & Loretz GmbH	Wax ointment	21000337002	7
Caesar & Loretz GmbH	Wax ointment	21002596001	8
Caesar & Loretz GmbH	Wax ointment	21002596002	1
Caesar & Loretz GmbH	Wax ointment	21003702002	1
Caesar & Loretz GmbH	Wax ointment	21003702003	3
Caesar & Loretz GmbH	Wax ointment	22001707001	1
Caesar & Loretz GmbH	Wax ointment	22002672001	3
Caesar & Loretz GmbH	Wax ointment	23000483001	3
Caesar & Loretz GmbH...	Wax ointment	19040002	1
Caesar & Loretz GmbH...	Wax ointment	21002596001	1
Caesar & Loretz GmbH...	Wax ointment	19000783001	1
Caesar & Loretz GmbH...	Wax ointment	19190501	1
Caesar & Loretz GmbH/Gehe	Wax ointment	19000783001	1
Caesar & Loretz GmbH/Gehe	Wax ointment	20002322001	2
Caesar & Loretz GmbH/Gehe	Wax ointment	20003013002	1
Caesar & Loretz GmbH...	Wax ointment	19040002	1
Caesar & Loretz GmbH...	Wax ointment	21000337002	1
Caesar & Loretz GmbH/Kehr	Wax ointment	19000783001	1
Caesar & Loretz GmbH...	Wax ointment	19000783001	1
Caesar & Loretz GmbH...	Wax ointment	21000337002	1
Caesar & Loretz GmbH...	Wax ointment	19000783001	1
Caesar & Loretz GmbH...	Wax ointment	20002322001	1
Caesar & Loretz GmbH...	Wax ointment	19000783001	1
Caesar & Loretz GmbH...	Wax ointment	19040002	1
Caesar & Loretz GmbH...	Wax ointment	19190501	2
Caesar & Loretz GmbH...	Wax ointment	190007840	1
Caesar & Loretz GmbH...	Wax ointment	19040001	3
Caesar & Loretz GmbH...	Wax ointment	19040002	1
Caesar & Loretz GmbH...	Wax ointment	22001707001	1
Caesar & Loretz GmbH...	Wax ointment	19000784002	3
Caesar & Loretz GmbH...	Wax ointment	20002322002	1
Caesar und Loretz GmbH	Wax ointment	17015001	1
Caesar& Loretz GmbH	Wax ointment	21002596002	1
Cealo / Otto Geilenk...	Wax ointment	19000783001	1
Cealo	Wax ointment	19190501	1
Cealo/Noweda	Wax ointment	16133401	1
Cealo/Noweda	Wax ointment	19190501	1
Cealo/Sanacorp	Wax ointment	18034602	1
Celo	Wax ointment	15424402	1
Gehe	Wax ointment	13072102	1
Gehe	Wax ointment	14235901	1
Gehe	Wax ointment	16133401	1
GEHE	Wax ointment	17171401	1
Gehe	Wax ointment	20002322002	1
Gehe	Wax ointment	20003013002	3
Gehe	Wax ointment	24001166001	1
Hedinger GmbH &Co KG	Wax ointment	18034602	1

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Supplier	Substance	Batch	Spectra
Henry Lamotte Olis G. . .	Wax ointment	15424301	1
Jenne	Wax ointment	19000783001	1
Jenne	Wax ointment	21002596002	1
Jenne	Wax ointment	23002428001	2
Jenne	Wax ointment	24001166001	1
Noveda	Wax ointment	23000438001	1
Noweda	Wax ointment	17171401	1
Noweda	Wax ointment	19040002	1
Noweda	Wax ointment	19190501	1
Noweda	Wax ointment	23000483001	1
Pharmachem/Sanacorp	Wax ointment	18L18-To9-062847	2
Phoenix	Wax ointment	19000783001	1
Phoenix	Wax ointment	19000784002	3
Phoenix	Wax ointment	24001166001	1
Phönix	Wax ointment	18258501	1
Phönix	Wax ointment	21002596001	1
Phönix	Wax ointment	21003702003	1
Sanacoro W.E:06.03.1. . .	Wax ointment	17171401	1
Sanacorp	Wax ointment	12352501	1
Sanacorp	Wax ointment	14073701	1
Sanacorp	Wax ointment	15205402	2
Sanacorp	Wax ointment	17015001	1
Sanacorp	Wax ointment	17294202	1
Sanacorp	Wax ointment	18162202	4
Sanacorp	Wax ointment	23000484001	1
VDL;6,45EUR;21.10.14	Wax ointment	14235901	1

- 19 909 spectra from 1539 *Apo-Ident* customers from a total of 6250 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Wax ointment* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wax ointment* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	27 654
Type B	0	540	0	30 390
Type C	0	868	1	19 909

The substance/substance group *Wax ointment* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9615 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9564 %)	100.0000 % (> 98.8889 %)
Type C	100.0000 % (> 99.0582 %)	99.8849 % (> 99.5397 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31111	31111	0.00	33.25
31167	31167	0.00	34.39
31444	31444	0.00	34.40
31911	31911	0.00	29.35
31912	31912	0.00	37.57
36402	36402	0.00	30.95

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **White paraffin oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 32342-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

White paraffin oil; Oleum Vaselini album

Special notes

When selecting the *White paraffin oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
White paraffin oil	4	3	22

Second-stage model

For differentiation of the substance/substance group *White paraffin oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *White paraffin oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Deumavan [®] protection ointment neutral	10.15	—
Marjoram ointment	19.90	—
Neribas [®] fat ointment	21.10	—
Protegin [®] XN	23.87	—
Cottonwood ointment	25.15	—
Asche Basis [®] fat ointment	25.71	—
Wax ointment	39.93	—
Lygal [®] ointment base	46.75	—
Stomahesive [®] adhesive paste	72.50	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *White paraffin oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *White paraffin oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	White paraffin oil	162192	32342	40	20160729*
Caelo	White paraffin oil	15380806	32565	40	not required
Caelo	White paraffin oil	21001958	35598	50	20210622*
Caelo	White paraffin oil	23000154001	37454	30	not required

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *White paraffin oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 4 different batches.
- 27 774 spectra from a total of 596 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *White paraffin oil*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	White paraffin oil	14338604	32454	40
Caelo	White paraffin oil	21004217002	36584	40
Caelo	White paraffin oil	24001960001	38930	40
Caelo	White paraffin oil	14338604	32846	40

- 30 770 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 47 spectra from 31 *Apo-Ident* customers from 23 batches from the substance/substance group *White paraffin oil*.
- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
AHD	White paraffin oil	23000154001	3
	White paraffin oil	23000154004	4
	White paraffin oil	24001960001	4
	White paraffin oil	23000154001	1
	White paraffin oil	16219207	1
	White paraffin oil	17175501	2
	White paraffin oil	17175506	2
	White paraffin oil	17175509	1
	White paraffin oil	18226101	1
	White paraffin oil	18226104	1
	White paraffin oil	18226105	1
	White paraffin oil	190763002	1
	White paraffin oil	19076301	2
	White paraffin oil	19076302	2
	White paraffin oil	20002135004	1
	White paraffin oil	20004223002	3
Caesar & Loretz GmbH	White paraffin oil	21004217002	2
	White paraffin oil	21003724002	1
	White paraffin oil	17175509	1
	White paraffin oil	20002135003	1
	White paraffin oil	20002135004	1
	White paraffin oil	20004223002	1
	White paraffin oil	21001958002	1
	White paraffin oil	21002439002	2
	White paraffin oil	21004217002	1
	White paraffin oil	21004217002	1
	White paraffin oil	18226105	1
	White paraffin oil	16219204	1
	White paraffin oil	17175506	1
	White paraffin oil		1
	White paraffin oil	2300154001	1
	White paraffin oil		1

- 20 731 spectra from 1559 *Apo-Ident* customers from a total of 6329 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *White paraffin oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *White paraffin oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	160	0	27 774
Type B	0	160	0	30 770
Type C	0	47	0	20 731

The substance/substance group *White paraffin oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9618 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.0593 %)	100.0000 % (> 87.2340 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
32342	32342	0.00	15.17
32565	32565	0.00	17.60
35598	35598	0.00	19.21
37454	37454	0.00	19.78

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Wintergreen oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 30455-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Wintergreen oil; Oleum gaultheria procumbens

Special notes

When selecting the *Wintergreen oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Wintergreen oil	2	2	15

Second-stage model

For differentiation of the substance/substance group *Wintergreen oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Wintergreen oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Clove oil	265.10	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Wintergreen oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Wintergreen oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Wintergreen oil	5411006-117696	31543	60	not required
Taoasis	Wintergreen oil	1828-125286	32807	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 100 spectra of 2 reference samples from the substance/substance group *Wintergreen oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 2 different batches.
- 27 834 spectra from a total of 598 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for

model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Wintergreen oil*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Wintergreen oil	00129A27	34399	40
Taoasis	Wintergreen oil	1953-128607	33624	40
Taoasis	Wintergreen oil	1828-125286	32936	40
Taoasis	Wintergreen oil	1953-128607	33625	40

- 30 770 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 16 spectra from 13 *Apo-Ident* customers from 16 batches from the substance/substance group *Wintergreen oil*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Wintergreen oil	7281-16678	1
Caelo	Wintergreen oil	10318703	1
Caelo	Wintergreen oil	10318714	1
Caelo	Wintergreen oil	13099202	1
Caelo	Wintergreen oil	13099205	1
Caelo	Wintergreen oil	15087406	1
Primavera, Gehe	Wintergreen oil	172K27	1
Primavera	Wintergreen oil	200D28	1
Primavera	Wintergreen oil	666L30	1
Taoasis	Wintergreen oil		1
Taoasis	Wintergreen oil	1303-121125	1
Taoasis	Wintergreen oil	2170-291	1
Taoasis	Wintergreen oil	423121-90971	1
Taoasis	Wintergreen oil	5091-11954	1
Taoasis	Wintergreen oil	97540	1
Taoasis/Taoasis	Wintergreen oil	2387-7212	1

- 20 762 spectra from 1559 *Apo-Ident* customers from a total of 6336 batches from a further 166 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Wintergreen oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wintergreen oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	100	0	27 834
Type B	0	159	1	30 770
Type C	0	16	0	20 762

The substance/substance group *Wintergreen oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9621 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9565 %)	99.3750 % (> 97.5000 %)
Type C	100.0000 % (> 99.0613 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31543	31543	0.00	272.71
32807	32807	0.00	273.08

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Yarrow oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 33795-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Yarrow oil

Special notes

When selecting the *Yarrow oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]
AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Yarrow oil	3	4	0

Second-stage model

For differentiation of the substance/substance group *Yarrow oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Yarrow oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Citus oil	21.31	—
Myrtle oil	23.30	—
Marjoram oil	23.97	—
Hyssop oil	25.53	—
Ravintsara oil	25.59	—
Angelica root oil	31.92	—
Matricaria oil, morrocan	33.88	—
Cypress oil	37.27	—
Rosemary oil	38.72	—
Juniper berry oil	41.70	—
Frankincense oil	42.70	—
Spearmint oil	42.99	—
Camphor oil	44.19	—
Matricaria oil, roman	44.58	—
Dwarf pine oil	44.72	—
Sage oil	47.51	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Yarrow oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Yarrow oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Yarrow oil	00516E25	33795	40	not required
Taoasis	Yarrow oil	2041-316	33822	40	not required
Taoasis	Yarrow oil	14521-DE-P02	37650	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Yarrow oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 3 different batches.
- 27 814 spectra from a total of 597 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Yarrow oil*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Yarrow oil	00677E26	34174	40
Primavera	Yarrow oil	00197J26	34295	40
Taoasis	Yarrow oil	128700	33823	40
Taoasis	Yarrow oil	19276	38601	40

- 30 770 spectra from a total of 705 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Yarrow oil*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 20 778 spectra from 1559 *Apo-Ident* customers from a total of 6352 batches from a further 167 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Yarrow oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Yarrow oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	120	0	27 814
Type B	0	160	0	30 770
Type C	0	0	0	20 778

The substance/substance group *Yarrow oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9619 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9565 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.0752 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra ([Rule of Three](#) [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the [Mahalanobis distance](#) to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33795	33795	0.00	52.70
33822	33822	0.00	23.99
37650	37650	0.00	61.28

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 3.0-2026-01

Validated substance/substance group **Ylang-ylang oil**
Substance class BR APIs & excipients, liquid/semi-solid (other)
Report date 28/04/2026
Report number 31506-2026-04-28
Executing company HiperScan GmbH
Gerokstraße 13
01307 Dresden
Germany

Relevant substance names

Ylang-ylang oil; Oleum ylang-ylang

Special notes

When selecting the *Ylang-ylang oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5 *European Pharmacopoeia 11th Edition, Basic Version 2022* [3]

Komm2.2.40 *Erfüllung von Ph. Eur. 2.2.40 durch Apo-Ident* [4]

AA010 *Creation of IdentModule Updates*

Validation method

Validation is performed after every change to the chemometric model (also “database”) in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ylang-ylang oil	5	3	0

Second-stage model

For differentiation of the substance/substance group *Ylang-ylang oil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ylang-ylang oil* in the substance class *BR APIs & excipients, liquid/semi-solid (other)*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.

A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.

Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Clary sage oil	30.15	—
Petitgrain oil	48.97	—
Lavender oil	59.38	—

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ylang-ylang oil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded under the control of *HiperScan GmbH* from traceable samples are used for the generation of the [chemometric models](#). The following samples have been obtained from the substance/substance group *Ylang-ylang oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Ylang-ylang oil	00403M26	34382	40	not required
Taoasis	Ylang-ylang oil	140114-115612	31506	60	not required
Taoasis	Ylang-ylang oil	07122-119828	31653	60	not required
Taoasis	Ylang-ylang oil	41813-124965	32808	40	not required
Taoasis	Ylang-ylang oil	17064	37675	40	not required

Validation samples

A total of 79 642 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Ylang-ylang oil*. These samples are listed above in the [calibration samples](#) section. The reference samples come from 5 different batches.

- 27694 spectra from a total of 595 batches from further 143 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix A](#). The samples in [Appendix A](#) were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out under the control of *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a [†]. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Ylang-ylang oil*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Ylang-ylang oil	01139K31	37979	40
Taoasis	Ylang-ylang oil	43197-126348	33049	40
Taoasis	Ylang-ylang oil	B966015-128199	33648	40

- 30810 spectra from a total of 706 batches from further 210 substances. These spectra were recorded under the control of *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix B](#).

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ylang-ylang oil*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 20778 spectra from 1559 *Apo-Ident* customers from a total of 6352 batches from a further 167 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Ylang-ylang oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ylang-ylang oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following

table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	240	0	27 694
Type B	0	92	28	30 810
Type C	0	0	0	20 778

The substance/substance group *Ylang-ylang oil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9616 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9566 %)	76.6667 % (> 74.1667 %)
Type C	100.0000 % (> 99.0752 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31506	31506	0.00	85.49
31653	31653	0.00	39.89
32808	32808	0.00	72.99
34382	34382	0.00	66.86
37675	37675	0.00	89.46

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

Appendix A: Additional calibration samples (*Type A*)

Substance spectra also enter the generation of the [chemometric model](#) which cannot be identified with this model. This serves the purpose that substances which the model is not supposed to recognise are safely rejected. The spectra of these samples are entered into the validation as *Type A*. They were recorded under the control of *HiperScan GmbH*.

The samples originate from 228 batches. From these, 10 159 spectra were recorded. The calibration spectra of substances which can be identified with the model are listed respectively in the section *calibration samples* for the individual substances and do not appear again elsewhere in this list.

0 A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

Supplier	Substance	Batch	Spectra	Certificate
Actavis	Abitima [®] clinic body cream	110712	40	not required
Actavis	Abitima [®] clinic body cream	051112	40	not required
Actavis	Abitima [®] clinic body cream	070915	40	not required
Actavis	Abitima [®] clinic body cream	331017	40	not required
PUREN Phar...	Abitima [®] clinic body cream	185393	40	not required
Actavis	Abitima [®] clinic face cream	46820	40	not required
Actavis	Abitima [®] clinic face cream	158584	40	not required
Actavis	Abitima [®] clinic face cream	161464	40	not required
Actavis	Abitima [®] clinic face cream	170180	40	not required
PUREN Phar...	Abitima [®] clinic face cream	22101318	40	not required
Allergika	ALLERGIKA [®] – Evening primose oil cream 20% MED	1504021	60	not required
Allergika	ALLERGIKA [®] – Evening primose oil cream 20% MED	1511051	60	not required
Allergika	ALLERGIKA [®] – Evening primose oil cream 20% MED	1609043	40	not required
Allergika	ALLERGIKA [®] – Evening primose oil cream 20% MED	2310101	40	not required
Allergika	ALLERGIKA [®] – Eyelid cream MED	2103030	40	not required
Allergika	ALLERGIKA [®] – Eyelid cream MED	2007042	40	not required
Allergika	ALLERGIKA [®] – Eyelid cream MED	2310090	40	not required
Allergika	ALLERGIKA [®] – Face cream MED	2104020	40	not required
Allergika	ALLERGIKA [®] – Face cream MED	2102013	40	not required
Allergika	ALLERGIKA [®] – Face cream MED	2304040	40	not required
Allergika	ALLERGIKA [®] -Lipolotio urea 5% F	1205050	80	not required
Allergika	ALLERGIKA [®] -Lipolotio urea 5% F	13112021	60	not required
Allergika	ALLERGIKA [®] -Lipolotio urea 5% F	1801022	40	not required
Allergika	ALLERGIKA [®] -Lipolotio urea 5% F	2011033	50	not required
Allergika	ALLERGIKA [®] -Lipolotio urea 5% F	2309050	40	not required
Almirall	Amciderm [®] Base cream	313311	60	not required
Almirall	Amciderm [®] Base cream	313311	75	not required
Almirall	Amciderm [®] Base cream	650341	40	not required
Almirall	Amciderm [®] Base cream	048171	40	not required
Caelo	Argan oil	161443	60	–*
Caelo	Argan oil	16035101	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
Chiesi	Asche Basis [®] cream	03117A	40	not required
Chiesi	Asche Basis [®] cream	22197A	40	not required
Chiesi	Asche Basis [®] cream	24220A	40	not required
Chiesi	Asche Basis [®] cream	14017A	40	not required
Chiesi	Asche Basis [®] fat ointment	23014A	40	not required
Chiesi	Asche Basis [®] fat ointment	41017A	60	not required
Chiesi	Asche Basis [®] fat ointment	53021A	40	not required
Chiesi	Asche Basis [®] fat ointment	02004A	40	not required
Chiesi	Asche Basis [®] lotion	21042A	40	not required
Chiesi	Asche Basis [®] lotion	24049A	40	not required
Chiesi	Asche Basis [®] lotion	64082A	40	not required
Chiesi	Asche Basis [®] ointment	21038A	40	not required
Chiesi	Asche Basis [®] ointment	21038A	40	not required
Chiesi	Asche Basis [®] ointment	21038A	40	not required
Chiesi	Asche Basis [®] ointment	13004A	40	not required

B

Supplier	Substance	Batch	Spectra	Certificate
Taoasis	Balm Bio Nature	150422-5106	60	not required
Taoasis	Balm Bio Nature	150422-5106	60	not required
Taoasis	Balm Bio Nature	151210-5337	40	not required
Taoasis	Balm Bio Nature	180515-8060	40	not required
Koko	Base cream DVL-P	L061S22	40	not required
Koko	Base cream DVL-P	L083T22	40	not required
Taoasis	Base cream Taoasis	121205-2276	100	not required
Taoasis	Base cream Taoasis	130124-3021	40	not required
Taoasis	Base cream Taoasis	141222-4350	60	not required
Taoasis	Base cream Taoasis	SAP4104-4030	30	not required

D

Supplier	Substance	Batch	Spectra	Certificate
P&M Cosmetics	Dermatest base ointment	251115	60	not required
P&M Cosmetics	Dermatest base ointment	180317	60	not required
P&M Cosmetics	Dermatest base ointment	121217	40	not required
P&M Cosmetics	Dermatest base ointment	040622	40	not required
P&M Cosmetics	Dermatest base ointment	270623	40	not required
P&M Cosmetics	Dermatest base ointment	301124	40	not required
Sanofi aventis	Dermatop [®] base cream	3F031A	40	not required
Sanofi aventis	Dermatop [®] base cream	5F056A	40	not required
Sanofi aventis	Dermatop [®] base cream	1F107A	40	not required
Sanofi aventis	Dermatop [®] base ointment	3F052A	40	not required
Sanofi aventis	Dermatop [®] base ointment	5F080A	60	not required
Sanofi aventis	Dermatop [®] base ointment	1F151A	40	not required
Allergika	Dermifant [®] kids cream 20% MED	1210082	80	not required
Allergika	Dermifant [®] kids cream 20% MED	1303033	40	not required
Allergika	Dermifant [®] kids cream 20% MED	1705043	40	not required
Allergika	Dermifant [®] kids cream 20% MED	2103037	50	not required
Allergika	Dermifant [®] kids cream 20% MED	2306040	40	not required
Kaymogyn GmbH	Deumavan [®] protection ointment neutral	41920120	40	not required
Kaymogyn GmbH	Deumavan [®] protection ointment neutral	13781119	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
Kaymogyn GmbH	Deumavan [®] protection ointment neutral	31660422	40	not required
Pierre Fabre	Dexeryl [®]	G99016	60	not required
Pierre Fabre	Dexeryl [®]	G00419	60	not required
Pierre Fabre	Dexeryl [®]	G00650	40	not required
Pierre Fabre	Dexeryl [®]	G00748	40	not required
Pierre Fabre	Dexeryl [®]	3GFF0	40	not required
Koko	DMS [®] base cream classic	L026G13	40	not required
Koko	DMS [®] base cream classic	L034H15	60	not required
Koko	DMS [®] base cream classic	L003H16	40	not required
Koko	DMS [®] base cream classic	L009K17	40	not required
Koko	DMS [®] base cream classic	L002F22	40	not required
Koko	DMS [®] base cream high classic	L010K13	70	not required
Koko	DMS [®] base cream high classic	L032A14	40	not required
Koko	DMS [®] base cream high classic	L041K15	60	not required
Koko	DMS [®] base cream high classic	L014H22	40	not required
Koko	DMS [®] base cream high classic plus	L014L13	40	not required
Koko	DMS [®] base cream high classic plus	L003L15	40	not required
Koko	DMS [®] base cream high classic plus	L103E22	40	not required

E

Supplier	Substance	Batch	Spectra	Certificate
Spirig Pharma	Excipial [®] almond oil ointment	N012	40	not required
Spirig Pharma	Excipial [®] almond oil ointment	R012	60	not required
Galderma L...	Excipial [®] hydro cream	0767004	50	not required
Galderma L...	Excipial [®] hydro cream	D492	40	not required
Spirig Pharma	Excipial [®] hydro cream	I013	40	not required
Spirig Pharma	Excipial [®] hydro cream	N013	40	not required
Spirig Pharma	Excipial [®] hydro cream	T052	40	not required
Galderma L...	Excipial [®] lipo cream	V051	40	not required
Galderma L...	Excipial [®] lipo cream	1769001	50	not required
Spirig Pharma	Excipial [®] lipo cream	I011	40	not required
Spirig Pharma	Excipial [®] lipo cream	N017	40	not required
Spirig Pharma	Excipial [®] lipo cream	R011	60	not required
Spirig Pharma	Excipial [®] lipo cream	T081	40	not required
Galderma L...	Excipial [®] U Hydrolotio	331554	40	not required
Galderma L...	Excipial [®] U Hydrolotio	365111	40	not required
Spirig Pharma	Excipial [®] U Hydrolotio	M016	40	not required
Spirig Pharma	Excipial [®] U Hydrolotio	M063	40	not required
Spirig Pharma	Excipial [®] U Hydrolotio	N013	40	not required
Spirig Pharma	Excipial [®] U Hydrolotio	R014	60	not required
Bios Medic...	Excipial [®] U Lipolotio	334288	50	not required
Galderma L...	Excipial [®] U Lipolotio	T122	40	not required
Spirig Pharma	Excipial [®] U Lipolotio	M042	60	not required
Spirig Pharma	Excipial [®] U Lipolotio	N031	40	not required
Spirig Pharma	Excipial [®] U Lipolotio	N085	40	not required
Galderma L...	Excipial [®] U10 Lipolotio	375347	40	not required
Spirig Pharma	Excipial [®] U10 Lipolotio	M021	60	not required

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Supplier	Substance	Batch	Spectra	Certificate
Spirig Pharma	Excipial [®] U10 Lipolotio	N025	40	not required
Spirig Pharma	Excipial [®] U10 Lipolotio	N047	40	not required

F

Supplier	Substance	Batch	Spectra	Certificate
Fontapharm	Fabitol [®] base cream	6RWW2	40	not required
Fontapharm	Fabitol [®] base cream	GWWL3	60	not required
Fontapharm	Fabitol [®] base cream	GLWD5	40	not required
Fontapharm	Fabitol [®] base cream	052002	50	20200508

H

Supplier	Substance	Batch	Spectra	Certificate
Hans Karre...	Hans Karrer Hydrocream MicroSilver	16001	40	not required
Hans Karre...	Hans Karrer Hydrocream MicroSilver	16002	40	not required
Hans Karre...	Hans Karrer Hydrocream MicroSilver	18002	40	not required
Hans Karre...	Hans Karrer Hydrocream MicroSilver	22004	40	not required
Hans Karre...	Hans Karrer Hydrocream MicroSilver	22002	40	not required
Hans Karre...	Hans Karrer Lipocream MicroSilver	15003	40	not required
Hans Karre...	Hans Karrer Lipocream MicroSilver	15005	40	not required
Hans Karre...	Hans Karrer Lipocream MicroSilver	18002	40	not required
Hans Karre...	Hans Karrer Lipocream MicroSilver	21002	50	not required
Hans Karre...	Hans Karrer Lipocream MicroSilver	22001	40	not required
Hans Karre...	Hans Karrer Lipolotion MicroSilver	15003	60	not required
Hans Karre...	Hans Karrer Lipolotion MicroSilver	15008	60	not required
Hans Karre...	Hans Karrer Lipolotion MicroSilver	18005	40	not required
Hans Karre...	Hans Karrer Lipolotion MicroSilver	22008	40	not required
Hans Karre...	Hans Karrer Lipolotion MicroSilver	22007	40	not required

L

Supplier	Substance	Batch	Spectra	Certificate
Licca Klin...	Licca base ointment	HR1310926	50	not required
Dr. Wolff	Linola [®] body milk	433240	60	not required
Dr. Wolff	Linola [®] body milk	511750	60	not required
Dr. Wolff	Linola [®] body milk	707930	40	not required
Dr. Wolff	Linola [®] body milk	D43639	40	not required
Astellas Pharma	Locobase [®] Protect	12B11/77	54	not required
Astellas Pharma	Locobase [®] Protect	13D06/75	40	not required
Astellas Pharma	Locobase [®] Protect	15I46/79	60	not required
Astellas Pharma	Locobase [®] Protect	16D35/77	40	not required
Karo Pharm...	Locobase [®] Protect	20I48/79	40	not required
Karo Pharm...	Locobase [®] Protect	21K41/77	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
Karo Pharm...	Locobase [®] Protect	130225	40	not required
Astellas Pharma	Locobase [®] Repair	12F18/77	55	not required
Astellas Pharma	Locobase [®] Repair	13E16/76	40	not required
Astellas Pharma	Locobase [®] Repair	16G60/75	40	not required
Karo Pharm...	Locobase [®] Repair	20G23/77	40	not required
Karo Pharm...	Locobase [®] Repair	22H11A	40	not required
Karo Pharm...	Locobase [®] Repair	24JM1B	40	not required
LEO Pharma GmbH	Locobase [®] Repair	17E20/75	40	not required
Almirall	Lygal [®] ointment base	222801	40	not required
Taurus	Lygal [®] ointment base	121302P	40	not required
Taurus	Lygal [®] ointment base	154841	40	not required
Taurus	Lygal [®] ointment base	164201	40	not required
Taurus	Lygal [®] ointment base	164201	40	not required
Taurus	Lygal [®] ointment base	164201	40	not required

M

Supplier	Substance	Batch	Spectra	Certificate
Ichthyol	Milk Cordes [®] O/W Emulsion	21D0006	40	not required
Ichthyol	Milk Cordes [®] O/W Emulsion	22D0014	40	not required
Ichthyol	Milk Cordes [®] O/W Emulsion	24D0008	40	not required

N

Supplier	Substance	Batch	Spectra	Certificate
Intendis	Neribas [®] cream	21076A	40	not required
Intendis	Neribas [®] cream	21076A	40	not required
Intendis	Neribas [®] cream	21076A	40	not required
Jenapharm	Neribas [®] fat ointment	32032C	40	not required
Jenapharm	Neribas [®] fat ointment	YY00K7C	60	not required
Jenapharm	Neribas [®] fat ointment	YY01TF2	40	not required
Bayer	Neribas [®] ointment	21053B	40	not required
Bayer	Neribas [®] ointment	21053B	40	not required
Jenapharm	Neribas [®] ointment	31064C	40	not required
Karo Pharm...	Neribas [®] ointment	YY04T3L	40	not required
Infectopharm	Neuroderm [®] care lotion	S041204.1	40	not required
Infectopharm	Neuroderm [®] care lotion	S031505.1	60	not required
Infectopharm	Neuroderm [®] care lotion	S071706.1	40	not required
Infectopharm	Neuroderm [®] care lotion	S042106.1	40	not required
Infectopharm	Neuroderm [®] care lotion	S052215.1	30	not required
Infectopharm	Neuroderm [®] care lotion	S122225.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream	S041214.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream	S021307.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream	S101428.1	60	not required
Infectopharm	Neuroderm [®] moisturising cream	S102210.1	30	not required
Infectopharm	Neuroderm [®] moisturising cream	S112119.1	30	not required
Infectopharm	Neuroderm [®] moisturising cream	S102218.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream lipo	S031202.1	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
Infectopharm	Neuroderm [®] moisturising cream lipo	S031506.1	60	not required
Infectopharm	Neuroderm [®] moisturising cream lipo	S051723.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream lipo	S072214.1	30	not required
Infectopharm	Neuroderm [®] moisturising cream lipo	S082224.1	30	not required

P

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Protegin [®] XN	13081901	40	not required
Caelo	Protegin [®] XN	13344402	40	not required
Caelo	Protegin [®] XN	17258703	40	not required
Caelo	Protegin [®] XN	24001198	40	20240514*

R

Supplier	Substance	Batch	Spectra	Certificate
Retterspitz...	Retterspitz external	016100	40	not required
Retterspitz...	Retterspitz external	017058	40	not required
Retterspitz...	Retterspitz external	016240	40	not required

S

Supplier	Substance	Batch	Spectra	Certificate
Devesa	Sebexol [®] basic pH 5 formula basis	1307	40	1403098
Devesa	Sebexol [®] basic pH 5 formula basis	1522	60	not required
Devesa	Sebexol [®] basic pH 5 formula basis	1638124	40	not required
Devesa	Sebexol [®] cream lotion	1220	40	1403097
Devesa	Sebexol [®] cream lotion	1317	40	not required
Devesa	Sebexol [®] cream lotion	1412	45	not required
Devesa	Sebexol [®] cream lotion	1531	60	not required
Devesa	Sebexol [®] cream lotion	1552.2	40	not required
Devesa	Sebexol [®] cream lotion	2128114	40	not required
ConvaTec Inc.	Stomahesive [®] adhesive paste	2D117	80	not required
ConvaTec Inc.	Stomahesive [®] adhesive paste	2M084	40	not required
ConvaTec Inc.	Stomahesive [®] adhesive paste	6L039	40	not required
Fagron	SyrSpend [®] SF pH4 cherry aroma	1503D017	60	not required
Fagron	SyrSpend [®] SF pH4 cherry aroma	1503D017	60	not required
Fagron	SyrSpend [®] SF pH4 cherry aroma	1704492/1	40	not required
Fagron	SyrSpend [®] SF pH4 aroma free	1503D009	60	not required
Fagron	SyrSpend [®] SF pH4 aroma free	1412D002	60	not required
Fagron	SyrSpend [®] SF pH4 aroma free	19011410	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
Fagron	SyrSpend [®] SF pH4 aroma free	22H11-T10-099025	40	not required
Fagron	SyrSpend [®] SF pH4 aroma free	24G11-T03-115196	40	not required

U

Supplier	Substance	Batch	Spectra	Certificate
Bayer	Ultrasicc [®]	33614A	40	not required
Hecht Phar...	Ultrasicc [®]	43382	40	not required

W

Supplier	Substance	Batch	Spectra	Certificate
Infectopharm	Wart InfectoPharm [®] 11.31)	ointment (NRF S031201.1	40	not required
Infectopharm	Wart InfectoPharm [®] 11.31)	ointment (NRF S031201.1	40	not required
Infectopharm	Wart InfectoPharm [®] 11.31)	ointment (NRF S121103.1	40	not required
Infectopharm	Wart InfectoPharm [®] 11.31)	ointment (NRF S112001.1	40	not required

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Appendix B: Additional validation samples (*Type B*)

It is necessary that spectra also enter the validation which cannot be identified with this model. In this manner, it is verified that the model also rejects unknown substances. The spectra for these samples were recorded under the control of *HiperScan GmbH*. They are allocated to the *Type B*. They also include the calibration spectra for other models.

The samples originate from 381 batches. From these 15 905 spectra were recorded. The spectra recorded on independent samples of substances which can be identified with the model are listed respectively in the section *Type B* for the individual substances and do not appear again elsewhere in this list.

0 A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

Supplier	Substance	Batch	Spectra	Certificate
Caelo	alpha-bisabolol (racemic) at least 85%	13360114	60	not required
Caelo	alpha-bisabolol (racemic) at least 85%	13360114	60	not required
Caelo	alpha-bisabolol (racemic) at least 85%	16271902	40	not required
Caelo	alpha-bisabolol (racemic) at least 85%	17065801	40	not required
Caelo	alpha-bisabolol (racemic) at least 85%	180585	40	20180214*
Koko	dermaividuals [®] base gel	L003L13	60	not required

A

Supplier	Substance	Batch	Spectra	Certificate
Actavis	Abitima [®] clinic body cream	072013	40	not required
Actavis	Abitima [®] clinic body cream	040116	40	not required
Actavis	Abitima [®] clinic body cream	040116	40	not required
Actavis	Abitima [®] clinic body cream	150818	40	not required
Actavis	Abitima [®] clinic body lotion	145054	40	not required
Actavis	Abitima [®] clinic body lotion	159997	40	not required
Actavis	Abitima [®] clinic body lotion	159997	40	not required
Actavis	Abitima [®] clinic face cream	158584	40	not required
Actavis	Abitima [®] clinic face cream	158584	40	not required
Allergika	ALLERGIKA [®] – Base cream	11/082022	40	not required
Allergika	ALLERGIKA [®] – Base cream	10/082022	40	not required
Allergika	ALLERGIKA [®] – Base cream	09/072022	40	not required
Allergika	ALLERGIKA [®] – Base cream	03/052026	40	not required
Allergika	ALLERGIKA [®] – Base cream	14/102023	40	not required
Allergika	ALLERGIKA [®] – Base cream	08/102025	40	not required
Allergika	ALLERGIKA [®] – Base ointment	03/052025	40	not required
Allergika	ALLERGIKA [®] – Base ointment	12/102023	40	not required
Allergika	ALLERGIKA [®] – Base ointment	05/062025	40	not required
Allergika	ALLERGIKA [®] – Evening primrose oil cream 20% MED	1607031	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
Allergika	ALLERGIKA [®] – Evening primrose oil cream 20% MED	1410062	40	not required
Allergika	ALLERGIKA [®] – Evening primrose oil cream 20% MED	2103051	50	not required
Allergika	ALLERGIKA [®] – Eyelid cream MED	2102010	40	not required
Allergika	ALLERGIKA [®] – Face cream MED	2102020	40	not required
Allergika	ALLERGIKA [®] -Lipolotio urea 5% F	1502011	40	not required
Allergika	ALLERGIKA [®] -Lipolotio urea 5% F	1502011	40	not required
Caelo	Aloe vera gel, 1:1	13025802	40	not required
Caelo	Aloe vera gel, 1:1	15329203	60	not required
Caelo	Aloe vera gel, 1:1	153292	60	20151111*
Caelo	Aloe vera gel, 1:1	153292	60	20151111*
Caelo	Aloe vera gel, 1:1	162489	40	20160907*
Caelo	Aloe vera gel, 1:1	162912	40	20161018*
Caelo	Aloe vera gel, 1:1	171341	40	20170516*
Caelo	Aloe vera gel, 1:1	172891	40	20171023*
Caelo	Aloe vera gel, 1:1	172890	40	20171025*
Caelo	Aloe vera gel, 1:1	181943	40	20180711*
Caelo	Aloe vera gel, 1:1	191914	40	20190718*
Caelo	Aloe vera gel, 1:1	21002409	50	20210830*
Caelo	Aloe vera gel, 1:1	22001060	40	20220407*
Caelo	Aloe vera gel, 1:1	22002254	40	20220722*
Caelo	Aloe vera gel, 1:1	23000170	40	20230222*
Caelo	Aloe vera gel, 1:1	23000170	10	20230222*
Caelo	Aloe vera gel, 1:1	23001282	40	20230601*
Almirall	Amciderm [®] Base cream	538331	40	not required
Almirall	Amciderm [®] Base cream	822351	40	not required
Dr. Wolff	Anefug [®] Simplex	234280	40	not required
Dr. Wolff	Anefug [®] Simplex	237590	40	1407216
Primavera	Anise seed oil	00480L26	40	not required
Caelo	Argan oil	16035101	40	not required
Caelo	Argan oil	162759	40	-*
Caelo	Argan oil	190980	40	20190412*
Chiesi	Asche Basis [®] cream	63351A	40	not required
Chiesi	Asche Basis [®] cream	63354A	40	not required
Chiesi	Asche Basis [®] cream	11002A	60	not required
Chiesi	Asche Basis [®] fat ointment	53021A	40	not required
Chiesi	Asche Basis [®] fat ointment	53021A	40	not required
Chiesi	Asche Basis [®] fat ointment	24010A	40	not required
Chiesi	Asche Basis [®] lotion	53075A	40	not required
Chiesi	Asche Basis [®] lotion	53075A	40	not required
Chiesi	Asche Basis [®] lotion	94106A	40	not required
Chiesi	Asche Basis [®] lotion	21007A	40	not required
Chiesi	Asche Basis [®] ointment	61067A	40	not required
Chiesi	Asche Basis [®] ointment	61067A	40	not required
Chiesi	Asche Basis [®] ointment	61067A	40	not required
Chiesi	Asche Basis [®] ointment	17072A	40	not required
Chiesi	Asche Basis [®] ointment	02089A	40	20200603

B

Supplier	Substance	Batch	Spectra	Certificate
Taoasis	Balm Bio Nature	160401-6083	40	not required
Taoasis	Balm Bio Nature	170403-7087	40	not required
Taoasis	Balm Bio Nature	0000004417	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
Koko	Base cream DVL-P	L021K22	40	not required
Taoasis	Base cream Taoasis	161124-6322	40	not required
Taoasis	Base cream Taoasis	161124-6322	40	not required
Taoasis	Base cream Taoasis	SAP3466-3139	40	not required
Bayer	Bepanthen [®] solution	KP08DR1	40	not required
Bayer	Bepanthen [®] solution	KP0ASHC	60	not required
Bayer	Bepanthen [®] solution	KP0B60L	40	not required
Bayer	Bepanthen [®] solution	KP0BJ61	40	not required
Bayer	Bepanthen [®] solution	KP0C3FU	40	not required
Bayer	Bepanthen [®] solution	KV02N2Z	40	not required
Bayer	Bepanthen [®] Wund- und Heilsalbe	GP00LB9	40	not required
Bayer	Bepanthen [®] Wund- und Heilsalbe	GP012SS	60	not required
Bayer	Bepanthen [®] Wund- und Heilsalbe	GP018T5	40	not required
Bayer	Bepanthen [®] Wund- und Heilsalbe	GP019ZF	40	not required
Bayer	Bepanthen [®] Wund- und Heilsalbe	GP01CTH	40	not required
Bayer	Bepanthen [®] Wund- und Heilsalbe	GP02287	40	not required
Taoasis	Black cumin oil	504511-115611	40	not required

C

Supplier	Substance	Batch	Spectra	Certificate
ASAV Apoth. ...	Common wormwood oil	10116310555	60	not required
ASAV Apoth. ...	Common wormwood oil	10815310556	40	not required
ASAV Apoth. ...	Common wormwood oil	10815310556	40	not required
ASAV Apoth. ...	Common wormwood oil	10815310556	40	not required
ASAV Apoth. ...	Common wormwood oil	10815310556	40	not required
ASAV Apoth. ...	Common wormwood oil	10409310558	40	not required
Taoasis	Common wormwood oil	7.9363	40	not required

D

Supplier	Substance	Batch	Spectra	Certificate
P&M Cosmetics	Dermatest base ointment	120911	40	not required
P&M Cosmetics	Dermatest base ointment	070615	20	not required
P&M Cosmetics	Dermatest base ointment	231115	40	not required
P&M Cosmetics	Dermatest base ointment	260820	40	not required
Fidia Phar. ...	Dermatop [®] base cream	2F112A	40	not required
Sanofi aventis	Dermatop [®] base cream	5F057A	40	not required
Sanofi aventis	Dermatop [®] base cream	7F069A	40	not required
Fidia Phar. ...	Dermatop [®] base ointment	3F167A	40	not required
Sanofi aventis	Dermatop [®] base ointment	5F089A	40	not required
Sanofi aventis	Dermatop [®] base ointment	7F106A	40	not required
Allergika	Dermifant [®] kids cream 20% MED	1607032	40	not required
Allergika	Dermifant [®] kids cream 20% MED	1801010	40	not required
Allergika	Dermifant [®] kids lotion	1301020	80	not required
Allergika	Dermifant [®] kids lotion	1306020	40	not required
Allergika	Dermifant [®] kids lotion	1607080	40	not required
Allergika	Dermifant [®] kids lotion	1705081	40	not required
Kaymogyn GmbH	Deumavan [®] protection ointment neutral	62170320	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
Pierre Fabre	Dexeryl [®]	G00623	40	not required
Pierre Fabre	Dexeryl [®]	G00658	40	not required
Koko	DMS [®] base cream classic	L003E16	40	not required
Koko	DMS [®] base cream classic	L003E16	40	not required
Koko	DMS [®] base cream classic	L077T22	40	not required
Koko	DMS [®] base cream classic	L052H22	40	not required
Koko	DMS [®] base cream high classic	L003H16	40	not required
Koko	DMS [®] base cream high classic	L037K16	40	not required
Koko	DMS [®] base cream high classic	L037K16	40	not required
Koko	DMS [®] base cream high classic	L064S22	40	not required
Koko	DMS [®] base cream high classic	L032K22	40	not required
Koko	DMS [®] base cream high classic plus	L018D16	40	not required
Koko	DMS [®] base cream high classic plus	L028T22	40	not required
Koko	DMS [®] base cream high classic plus	L110H022	40	not required
Primavera	Douglas fir oil	00539M26	40	not required

E

Supplier	Substance	Batch	Spectra	Certificate
Beiersdorf	Eucerinum O/W basis	41830108WA	60	not required
Beiersdorf	Eucerinum O/W basis	64030208WA	40	not required
Beiersdorf	Eucerinum O/W basis	64030208WA	40	not required
Beiersdorf	Eucerinum O/W basis	64030208WA	40	not required
Beiersdorf	Eucerinum O/W basis	94830308WA	40	not required
Beiersdorf	Eucerinum W/O basis	31230108WA	40	not required
Beiersdorf	Eucerinum W/O basis	53430208WA	40	not required
Beiersdorf	Eucerinum W/O basis	72630108WA	40	not required
Beiersdorf	Eucerinum W/O basis	72630108WA	40	not required
Beiersdorf	Eucerinum W/O basis	83730208WA	40	not required
Galderma L...	Excipial [®] almond oil ointment	1774011	50	not required
Galderma L...	Excipial [®] almond oil ointment	2774006	30	not required
Spirig Pharma	Excipial [®] almond oil ointment	M023	40	not required
Spirig Pharma	Excipial [®] almond oil ointment	M031	40	not required
Spirig Pharma	Excipial [®] almond oil ointment	S021	40	not required
Spirig Pharma	Excipial [®] almond oil ointment	T052	40	not required
Galderma L...	Excipial [®] hydro cream	1767002	40	not required
Spirig Pharma	Excipial [®] hydro cream	I013	40	not required
Spirig Pharma	Excipial [®] hydro cream	N013	40	not required
Spirig Pharma	Excipial [®] hydro cream	50235	40	not required
Galderma L...	Excipial [®] lipo cream	V051	40	not required
Galderma L...	Excipial [®] lipo cream	D372	40	not required
Spirig Pharma	Excipial [®] lipo cream	N017	40	not required
Spirig Pharma	Excipial [®] U Hydrolotio	S061	40	not required
Spirig Pharma	Excipial [®] U Hydrolotio	V052	40	not required
Galderma L...	Excipial [®] U Lipolotio	V011	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
Galderma L. . .	Excipial [®] U Lipolotio	371412	40	not required
Spirig Pharma	Excipial [®] U Lipolotio	T122	40	not required
Spirig Pharma	Excipial [®] U Lipolotio	T122	40	not required
Galderma L. . .	Excipial [®] U10 Lipolotio	339855	50	not required
Spirig Pharma	Excipial [®] U10 Lipolotio	T072	40	not required
Spirig Pharma	Excipial [®] U10 Lipolotio	50393	40	not required

F

Supplier	Substance	Batch	Spectra	Certificate
Fontapharm	Fabitop [®] base cream	GRWW1	40	not required
Fontapharm	Fabitop [®] base cream	GLWD4	40	not required
GSK Consum. . .	Fenistil [®] Gel	T02415A	40	not required
GSK Consum. . .	Fenistil [®] Gel	T02416A	40	not required
GSK Consum. . .	Fenistil [®] Gel	U02364A	40	not required
Novartis	Fenistil [®] Gel	N00927A	40	not required
Novartis	Fenistil [®] Gel	R02021A	60	not required
Fagron	Fitalite [™]	14B18-T01-010352	60	not required
Fagron	Fitalite [™]	14B18-T01-010352	60	not required
Fagron	Fitalite [™]	1503259	40	not required
Fagron	Fitalite [™]	1503259	40	not required
Fagron	Fitalite [™]	1503259	40	not required

G

Supplier	Substance	Batch	Spectra	Certificate
Pharmapol	Glycerol trinitrate 5%	228718	40	not required
Pharmapol	Glycerol trinitrate 5%	232961	60	not required

H

Supplier	Substance	Batch	Spectra	Certificate
Hans Karre. . .	Hans Karrer Hydrocream	16003	40	not required
Hans Karre. . .	MicroSilver			
Hans Karre. . .	Hans Karrer Hydrocream	16004	40	not required
Hans Karre. . .	MicroSilver			
Hans Karre. . .	Hans Karrer Hydrocream	21003	50	not required
Hans Karre. . .	MicroSilver			
Hans Karre. . .	Hans Karrer Lipocream Mi-	17001	40	not required
Hans Karre. . .	croSilver			
Hans Karre. . .	Hans Karrer Lipocream Mi-	16002	40	not required
Hans Karre. . .	croSilver			
Hans Karre. . .	Hans Karrer Lipocream Mi-	22002	40	not required
Hans Karre. . .	croSilver			
Hans Karre. . .	Hans Karrer Lipolotion Mi-	16005	40	not required
Hans Karre. . .	croSilver			
Hans Karre. . .	Hans Karrer Lipolotion Mi-	18004	40	not required
Hans Karre. . .	croSilver			
Hans Karre. . .	Hans Karrer Lipolotion Mi-	21008	50	not required
Hans Karre. . .	croSilver			
Primavera	Ho leaf oil	00388M26	40	not required

J

Supplier	Substance	Batch	Spectra	Certificate
Primavera	Jasmine 4% in alcohol	00184A27	40	not required

K

Supplier	Substance	Batch	Spectra	Certificate
Spirig Pharma	Kerasal [®] base ointment	M031	40	not required
Spirig Pharma	Kerasal [®] base ointment	N011	40	not required

L

Supplier	Substance	Batch	Spectra	Certificate
La Roche-Posay	La Roche-Posay Cold Cream Naturel	54J01P	40	not required
La Roche-Posay	La Roche-Posay Cold Cream Naturel	54K31P	40	not required
La Roche-Posay	La Roche-Posay Cold Cream Naturel	54LN1P	60	not required
La Roche-Posay	La Roche-Posay Cold Cream Naturel	54M51P	40	not required
La Roche-Posay	La Roche-Posay Cold Cream Naturel	54P61P	40	not required
La Roche-Posay	La Roche-Posay Toleriane	54J901	40	not required
La Roche-Posay	La Roche-Posay Toleriane	54K500	40	not required
La Roche-Posay	La Roche-Posay Toleriane	54N201	40	not required
La Roche-Posay	La Roche-Posay Toleriane	54N600	40	not required
La Roche-Posay	La Roche-Posay Toleriane	54P401	40	not required
Primavera	Lavandin oil	00508L26	40	not required
Primavera	Lemon verbena leaf oil	00540M26	40	not required
Dr. Wolff	Linola [®] acute 0.5%	334620	40	not required
Dr. Wolff	Linola [®] body milk	606430	40	not required
Dr. Wolff	Linola [®] body milk	609202	40	not required
Dr. Wolff	Linola [®] fat cream	235260	40	not required
Dr. Wolff	Linola [®] fat cream	337280	40	not required
Dr. Wolff	Linola [®] fat cream	603820	40	not required
Dr. Wolff	Linola [®] fat cream	611011	40	not required
Dr. Wolff	Linola [®] fat cream	612211	40	not required
Dr. Wolff	Linola [®] fat cream	607250	40	not required
Dr. Wolff	Linola [®] fat cream	802990	40	not required
Dr. Wolff	Linola [®] H fat N	333080	40	not required
Dr. Wolff	Linola [®] H fat N	603230	40	not required
Dr. Wolff	Linola [®] H fat N	611060	40	not required
Dr. Wolff	Linola [®] H fat N	611060	40	not required
Dr. Wolff	Linola [®] H fat N	801410	40	not required
Dr. Wolff	Linola [®] O/W cream	238482	40	not required
Dr. Wolff	Linola [®] O/W cream	334010	40	not required
Dr. Wolff	Linola [®] O/W cream	432480	40	not required
Dr. Wolff	Linola [®] Sept	334080	40	not required
Dr. Wolff	Linola [®] Sept	509361	60	not required
Dr. Wolff	Linola [®] Sept	603190	40	not required
Dr. Wolff	Linola [®] Sept	603190	40	not required
Dr. Wolff	Linola [®] Sept	707990	40	not required
Dr. Wolff	Linola [®] sun protection SPF 50 lotion	134530	40	not required
Spirig Pharma	Lipoderm [®] lotion	K057	40	not required
Spirig Pharma	Lipoderm [®] lotion	M065	40	not required
Spirig Pharma	Lipoderm [®] lotion	R023	60	not required
Spirig Pharma	Lipoderm [®] lotion	V012	40	not required
Spirig Pharma	Lipoderm [®] lotion	V042	40	not required
Primavera	Litsea oil	00496L26	40	not required
Astellas Pharma	Locobase [®] Protect	16D35/77	40	not required
Karo Pharm...	Locobase [®] Protect	24D78A	40	not required
Karo Pharm...	Locobase [®] Protect	270225	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
LEO Pharma GmbH	Locobase [®] Protect	17B27/75	40	not required
Astellas Pharma	Locobase [®] Repair	15K07/77	40	not required
Karo Pharm. ...	Locobase [®] Repair	24G68A	40	not required
Almirall	Lygal [®] head ointment N 3%	222212	40	not required
Taurus	Lygal [®] head ointment N 3%	124311	40	not required
Taurus	Lygal [®] head ointment N 3%	143710	60	not required
Taurus	Lygal [®] head ointment N 3%	160732	40	not required
Taurus	Lygal [®] head ointment N 3%	160732	40	not required
Taurus	Lygal [®] head ointment N 3%	181802	40	not required
Almirall	Lygal [®] ointment base	174104	40	not required
Taurus	Lygal [®] ointment base	124904P	60	not required

M

Supplier	Substance	Batch	Spectra	Certificate
Ichthyol	Milk Cordes [®] O/W Emulsion	22D0018	40	not required
Caelo	Milking grease Special without Osmaron [®]	162049	40	20160711*

N

Supplier	Substance	Batch	Spectra	Certificate
Jenapharm	Neribas [®] cream	YY01FX3	40	not required
Jenapharm	Neribas [®] cream	YY01X64	40	not required
Karo Pharm. ...	Neribas [®] cream	YY04EYL	40	not required
Karo Pharm. ...	Neribas [®] cream	24K77A	40	not required
Jenapharm	Neribas [®] fat ointment	YY011K0	40	not required
Jenapharm	Neribas [®] fat ointment	YY019KR	40	not required
Karo Pharm. ...	Neribas [®] fat ointment	YY04F1L	40	not required
Jenapharm	Neribas [®] ointment	YY00TJ0	40	not required
Jenapharm	Neribas [®] ointment	YY016EC	40	not required
Infectopharm	Neuroderm [®] care lotion	S111514.1	40	not required
Infectopharm	Neuroderm [®] care lotion	S081610.1	40	not required
Infectopharm	Neuroderm [®] care lotion	S052214.1	30	not required
Infectopharm	Neuroderm [®] care lotion	S112314.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream	S051612.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream	S051612.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream	S112119.1	20	not required
Infectopharm	Neuroderm [®] moisturising cream	S092318.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream lipo	S071617.2	40	not required
Infectopharm	Neuroderm [®] moisturising cream lipo	S021706.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream lipo	S022106.1	40	not required
Infectopharm	Neuroderm [®] moisturising cream lipo	S112322.1	40	not required

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Supplier	Substance	Batch	Spectra	Certificate

O

Supplier	Substance	Batch	Spectra	Certificate
Almirall	Optiderm [®] lotion	341431	40	not required
Almirall	Optiderm [®] lotion	511951	60	not required
Almirall	Optiderm [®] lotion	633771	20	not required
Almirall	Optiderm [®] lotion	706961	40	not required
Almirall	Optiderm [®] lotion	706961	40	not required
Paddock	Ora-Blend [®]	2280130	40	not required
Perrigo	Ora-Blend [®] SF	3112578	40	not required
Fagron	Ora-Plus [®]	3334081	60	not required
Perrigo	Ora-Plus [®]	3334081	40	not required
Fagron	Ora-Sweet [®]	3062252	40	not required
Perrigo	Ora-Sweet [®]	3062252	40	not required

P

Supplier	Substance	Batch	Spectra	Certificate
Winthrop	Panthenol ointment Lichtenstein	2290680H	40	not required
Winthrop	Panthenol ointment Lichtenstein	2290718H	40	not required
Zentiva Ph...	Panthenol ointment Lichtenstein	EH4594	60	not required
Zentiva Ph...	Panthenol ointment Lichtenstein	GC5567	40	not required
Zentiva Ph...	Panthenol ointment Lichtenstein	GD5661	40	not required
Caelo	Perfume oil vanilla	10293212	40	not required
Caelo	Perfume oil vanilla	13393501	40	1403100
Caelo	Perfume oil vanilla	13393501	40	not required
Caelo	Perfume oil vanilla	14284107	60	not required
Caelo	Perfume oil vanilla	15316308	40	not required
Caelo	Perfume oil vanilla	15316308	40	not required
Stiefel	Physiogel [®] hypoallergenic cream	343P	40	not required
Stiefel	Physiogel [®] hypoallergenic cream	6940	40	not required
Caelo	Pine oil rubbing alcohol	162091	40	20160713*
Stoko	Praecutan [®] lotion F	0915777806	40	not required
Stoko	Praecutan [®] lotion F	011657101571	40	not required
Caelo	Protegin [®] XN	161645	40	20160711*
Caelo	Protegin [®] XN	21003187003	40	20211028

R

Supplier	Substance	Batch	Spectra	Certificate
Retterspit...	Retterspitz external	016179	30	not required
Retterspit...	Retterspitz external	017192	40	not required
Einhorn-Ap...	Rizol raw material	AL0413-1	60	not required
Primavera	Rose oil 10%	00721716	40	not required

S

Supplier	Substance	Batch	Spectra	Certificate
Salderman ...	Salderman base emulsion	180123	40	not required
Salderman ...	Salderman base emulsion	220321-1	40	not required
Bombastus	Salicylic white paraffin 10%	287820	60	not required

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Supplier	Substance	Batch	Spectra	Certificate
Bombastus	Salicylic white paraffin 10%	291886	75	not required
Bombastus	Salicylic white paraffin 10%	302737	40	not required
Bombastus	Salicylic white paraffin 10%	309004	40	not required
Bombastus	Salicylic white paraffin 10%	310227	40	not required
Bombastus	Salicylic white paraffin 10%	22004053	40	not required
Caelo	Salmon oil	170345	40	20170213*
Caelo	Salmon oil	173079	40	20171116*
Caelo	Salmon oil	182524	40	20181005*
Caelo	Salmon oil	20000795	40	20200330*
Caelo	Salmon oil	21003192	50	20211015*
Caelo	Salmon oil	21004006	40	20211216*
Caelo	Salmon oil	24000368	40	20240223*
Primavera	Seabuckthorn oil, organic	00346E26	40	not required
Devesa	Sebexol [®] basic pH 5 for- mula basis	1712122	40	not required
Devesa	Sebexol [®] basic pH 5 for- mula basis	1644102	40	not required
Devesa	Sebexol [®] basic pH 5 for- mula basis	2243126	40	not required
Devesa	Sebexol [®] cream lotion	1605101	40	not required
Devesa	Sebexol [®] cream lotion	1605101	40	not required
Devesa	Sebexol [®] cream lotion	2338120	40	not required
Ichthyol	Solutio Cordes [®]	12B006	40	not required
Ichthyol	Solutio Cordes [®]	13B001	40	not required
Ichthyol	Solutio Cordes [®]	15B005	60	not required
Ichthyol	Solutio Cordes [®]	15B005	40	not required
Ichthyol	Solutio Cordes [®]	17B007	40	not required
Ichthyol	Solutio Cordes [®]	19B007	40	not required
Ichthyol	Solutio Cordes [®]	21B0003	50	not required
Ichthyol	Solutio Cordes [®]	22B0004	40	not required
Ichthyol	Solutio Cordes [®]	22B0003	40	not required
Primavera	Spanish sage oil	00057G26	40	not required
ConvaTec Inc.	Stomahesive [®] adhesive paste	6D079	40	not required
ConvaTec Inc.	Stomahesive [®] adhesive paste	5G062	40	not required
Fagron	SyrSpend [®] SF pH4 cherry aroma	1503255	40	not required
Fagron	SyrSpend [®] SF pH4 cherry aroma	1603252/2	40	not required
Fagron	SyrSpend [®] SF pH4 cherry aroma	23D05-T04-104277	40	not required
Fagron	SyrSpend [®] SF pH4 aroma free	1704493	40	not required
Fagron	SyrSpend [®] SF pH4 aroma free	1704493	40	not required

T

Supplier	Substance	Batch	Spectra	Certificate
Bene	Thrombocid [®] gel	401B101	40	not required
Bene	Thrombocid [®] gel	401B101	40	not required
Bene	Thrombocid [®] gel	403I143	40	not required
Bene	Thrombocid [®] gel	403I143	40	not required
Bene	Thrombocid [®] gel	403I143	40	not required
Bene	Thrombocid [®] ointment	410B113	40	not required
Bene	Thrombocid [®] ointment	410B113	40	not required
Bene	Thrombocid [®] ointment	408C141	40	not required
Bene	Thrombocid [®] ointment	409A151	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
Taoasis	Thuja oil	66255-969	40	not required
Taoasis	Thuja oil	28508-121881	40	not required
Taoasis	Thuja oil	66255-2932	40	not required
Taoasis	Tolu res. 50% oil	493887-105383BAC90451	40	not required
Primavera	Tolu Resinoid	00115A25	40	not required
Taoasis	Tonka extract	3636K08	40	not required

U

Supplier	Substance	Batch	Spectra	Certificate
Bayer	Ultrabas [®]	33851A	40	not required
Hecht Phar...	Ultrabas [®]	34069	40	not required
Bayer	Ultrapril [®]	22100A	40	not required
Hecht Phar...	Ultrasicc [®]	34837	40	not required
Caelo	Ultrasound contact gel	12031301	40	not required

V

Supplier	Substance	Batch	Spectra	Certificate
Taoasis	Vanilla extract oil	789171-114788	40	not required
Caelo	Vario base cream	12077902	50	1405329
Caelo	Vario base cream	13257102	40	1405330
Fagron	Versatile Anhydrous Cream Base	24F14-T03-114472	40	not required
Fagron	Versatile Anhydrous Cream Base	24J14-T08-117002	40	not required
Fagron	Versatile [™]	14B19-T02-010391	60	not required
Fagron	Versatile [™]	14B19-T02-010391	60	not required
Fagron	Versatile [™]	1503256	40	not required
Fagron	Versatile [™]	1503256	40	not required
Fagron	Versatile [™]	1503256	40	not required
Fagron	Versatile [™] Rich	14B19-T08-010395	60	not required
Fagron	Versatile [™] Rich	14B19-T04-010395	60	not required
Fagron	Versatile [™] Rich	1503257	40	not required
Fagron	Versatile [™] Rich	1503257	40	not required
Fagron	Versatile [™] Rich	1503257	40	not required

W

Supplier	Substance	Batch	Spectra	Certificate
Infectopharm	Wart InfectoPharm [®] 11.31)	ointment (NRF	S021601.1	40 not required
Infectopharm	Wart InfectoPharm [®] 11.31)	ointment (NRF	S071602.1	40 not required
Infectopharm	Wart InfectoPharm [®] 11.31)	ointment (NRF	S071602.1	40 not required
Infectopharm	Wart InfectoPharm [®] 11.31)	ointment (NRF	S061801.1	40 not required
Infectopharm	Wart InfectoPharm [®] 11.31)	ointment (NRF	S042201.1	40 not required
Infectopharm	Wart InfectoPharm [®] 11.31)	ointment (NRF	S082402.1	40 not required

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Appendix C: Additional validation samples (*Type C*)

Spectra for substances from the field which cannot be identified with this model also enter the validation. In this manner, it is verified that the model also rejects unknown substances. The spectra for these samples were recorded by *Apo-Ident* customers. They belong to *Type C*. The information provided by the customer regarding the manufacturer and batch number is taken over by *HiperScan GmbH* to a large extent unchecked.

The samples originate from 3518 batches. From these, 13 788 spectra were recorded. The spectra recorded on independent samples of substances from the field which can be identified with the model are listed respectively in the section *Type C* for the individual substances and do not appear again elsewhere in this list.

0 A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

Supplier	Substance	Batch	Spectra
Caelo	alpha-bisabolol (racemic) a...	14322713	1
Caelo	alpha-bisabolol (racemic) a...	18058503	1
Caelo	alpha-bisabolol (racemic) a...	18306002	1
Caelo	alpha-bisabolol (racemic) a...	18306001	2
Caelo	alpha-bisabolol (racemic) a...	18058504	1
Caelo	alpha-bisabolol (racemic) a...	18058506	2
Caesar & Loretz GmbH	alpha-bisabolol (racemic) a...	19000485002	1
Caesar & Loretz Gm...	alpha-bisabolol (racemic) a...	20004203002	1
Spangro 28.1.2019	alpha-bisabolol (racemic) a...	180580506	1
Spinnrad	alpha-bisabolol (racemic) a...	920303032	1

A

Supplier	Substance	Batch	Spectra
	Abitima [®] clinic body cream	185393	6
	Abitima [®] clinic body cream	186365	1
	Abitima [®] clinic body cream	186372	1
	Abitima [®] clinic body cream	194192	1
	Abitima [®] clinic body cream	196073	1
A.H.D.	Abitima [®] clinic body cream	260515	3
Abitima	Abitima [®] clinic body cream	52015/051112	1
Abitima / Gehe	Abitima [®] clinic body cream	251118	18
actavis	Abitima [®] clinic body cream	20912	3
actavis	Abitima [®] clinic body cream	70513	1
Actavis	Abitima [®] clinic body cream	31114	2
Actavis	Abitima [®] clinic body cream	10915	4
Actavis	Abitima [®] clinic body cream	32018	1
Actavis	Abitima [®] clinic body cream	131115	1
Actavis Deutschlan...	Abitima [®] clinic body cream	350313	2
Actavis Deutschlan...	Abitima [®] clinic body cream	31015	3
Actavis Deutschlan...	Abitima [®] clinic body cream	121115	1
Actavis/ Gehe	Abitima [®] clinic body cream	60513	4
actavis/Gehe	Abitima [®] clinic body cream	112015	1
Actavis/Gehe	Abitima [®] clinic body cream	51112	2
Actavis/Gehe	Abitima [®] clinic body cream	81013	1
Actavis/Noweda	Abitima [®] clinic body cream	21015	2
Actavis/Sanacorp	Abitima [®] clinic body cream	110712	5
APL Swift Services	Abitima [®] clinic body cream	92021	1
APL Swift, Noweda	Abitima [®] clinic body cream	20118	6
Astellas Pharma	Abitima [®] clinic body cream	190213	1
Caelo	Abitima [®] clinic body cream	40116	1
Caelo	Abitima [®] clinic body cream	100517	3
Gehe	Abitima [®] clinic body cream	186727	1

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Supplier	Substance	Batch	Spectra
GEHE	Abitima [®] clinic body cream	100116	2
GEHE	Abitima [®] clinic body cream	331017	2
Noweda/Actavis	Abitima [®] clinic body cream	90118	9
Fagron	Abitima [®] clinic body cream	110517	3
Fagron	Abitima [®] clinic body cream	241118	8
Puren Pharm/Phönix	Abitima [®] clinic body cream	1311118	1
Puren Pharma	Abitima [®] clinic body cream	130319	9
Puren Pharma / Kehr	Abitima [®] clinic body cream	18012G	1
Puren Pharma GmbH	Abitima [®] clinic body cream	131118	9
Puren Pharma GmbH	Abitima [®] clinic body cream	13118	1
Puren Pharma GmbH	Abitima [®] clinic body cream	180125	5
PUREN Pharma GmbH	Abitima [®] clinic body cream	2025-02	2
...			
Puren Pharma GmbH/...	Abitima [®] clinic body cream	120319	5
Puren Pharma/Anzag	Abitima [®] clinic body cream	180007	5
Puren Pharma/GEHE	Abitima [®] clinic body cream	120119	8
Puren Pharma/Phönix	Abitima [®] clinic body cream	185394	11
Puren Pharma/Sanacorp	Abitima [®] clinic body cream	180126	4
Puren/Gehe	Abitima [®] clinic body cream	185433	1
Puren/Phoenix	Abitima [®] clinic body cream	130118	1
Puren/Phoenix	Abitima [®] clinic body cream	261118	18
Roche/AHD	Abitima [®] clinic body cream	142620	1
Sanacorp	Abitima [®] clinic body cream	210612	1
Sanacorp	Abitima [®] clinic body cream	70512	1
Sanacorp	Abitima [®] clinic body cream	12015/110/12	1
Sanacorp	Abitima [®] clinic body cream	140113	2
Actavis/Alliance	Abitima [®] clinic body lotion	161613	1
	Abitima [®] clinic face cream	22101318	3
	Abitima [®] clinic face cream	21101203	2
	Abitima [®] clinic face cream	23100295	1
	Abitima [®] clinic face cream	23100296	1
	Abitima [®] clinic face cream	23101933	2
	Abitima [®] clinic face cream	23100346	2
	Abitima [®] clinic face cream	23102129	2
	Abitima [®] clinic face cream	23102163	2
	Abitima [®] clinic face cream	23102164	1
	Abitima [®] clinic face cream	23102165	3
actavis	Abitima [®] clinic face cream	148496	2
actavis	Abitima [®] clinic face cream	148495	2
actavis	Abitima [®] clinic face cream	150202	1
actavis	Abitima [®] clinic face cream	150203	2
Actavis	Abitima [®] clinic face cream	160670	1
Actavis / Anzag	Abitima [®] clinic face cream	148024	1
Actavis / Anzag	Abitima [®] clinic face cream	148503	1
Actavis / Anzag	Abitima [®] clinic face cream	150237	1
Actavis / Gehe	Abitima [®] clinic face cream	161904	3
Actavis / Noweda	Abitima [®] clinic face cream	142371	1
Actavis/ Gehe	Abitima [®] clinic face cream	164221	1
actavis/Gehe	Abitima [®] clinic face cream	164225	4
Actavis/GEHE	Abitima [®] clinic face cream	148051	1
Actavis/Noweda	Abitima [®] clinic face cream	161423	1
Actavis/Phönix	Abitima [®] clinic face cream	159274	2
APL Swift / Phoenix	Abitima [®] clinic face cream	171873	1
APL Swift Service	Abitima [®] clinic face cream	21101170	2
APL Swift/Gehe	Abitima [®] clinic face cream	20101761	1

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Supplier	Substance	Batch	Spectra
Caelo	Abitima [®] clinic face cream	149666	2
Caelo	Abitima [®] clinic face cream	161468	3
Caelo	Abitima [®] clinic face cream	170180	6
Dr. Wolff	Abitima [®] clinic face cream	15726	1
Fagron	Abitima [®] clinic face cream	150204	1
Gehe	Abitima [®] clinic face cream	211001203	1
Noweda	Abitima [®] clinic face cream	146735	2
Persano/Gehe	Abitima [®] clinic face cream	57792	1
Phoenix/actavis	Abitima [®] clinic face cream	148460	1
Puren	Abitima [®] clinic face cream	169356	1
Puren	Abitima [®] clinic face cream	22100373	8
Puren / Gehe	Abitima [®] clinic face cream	174292	5
Puren / Phoenix	Abitima [®] clinic face cream	22100374	3
Puren / Phönix	Abitima [®] clinic face cream	169357	2
Puren / Phönix	Abitima [®] clinic face cream	171872	1
Puren / Phönix	Abitima [®] clinic face cream	174418	4
Puren / Phönix	Abitima [®] clinic face cream	20101760	2
Puren / Sanacorp	Abitima [®] clinic face cream	22100405	3
Puren Pharma	Abitima [®] clinic face cream	211001192	1
Puren Pharma/ Gehe...	Abitima [®] clinic face cream	21101217	2
Puren/Gehe	Abitima [®] clinic face cream	20101613	1
Allergika Basiscre...	ALLERGIKA [®] – Base cream	11062023	1
Allergika Pharma GmbH	ALLERGIKA [®] – Base cream		4
allergika pharma g...	ALLERGIKA [®] – Base cream	8/072024	1
Allergika Pharma G...	ALLERGIKA [®] – Base cream	9/102025	1
Allergika Pharma G...	ALLERGIKA [®] – Base cream	11/112025	1
Allergika Pharma/S...	ALLERGIKA [®] – Base cream	2012023	1
Allergika/ GEHE	ALLERGIKA [®] – Base cream	2/012023	1
Allergika/Phönix	ALLERGIKA [®] – Base cream	4/032023	1
Henry Lamotte / 2	ALLERGIKA [®] – Base cream	14/102023	1
Kehr 22.09.2020	ALLERGIKA [®] – Base cream	2/2025	1
	ALLERGIKA [®] – Evening primos...	2310100	1
	ALLERGIKA [®] – Evening primos...	2403040	1
	ALLERGIKA [®] – Eyelid cream MED	2305041	1
ALLERGIKA Pharma GmbH	ALLERGIKA [®] – Face cream MED	2/022027	1
Allergika Pharma GmbH	ALLERGIKA [®] -Lipolotio urea 5% F	1502011	1
Allergika/Ebert	ALLERGIKA [®] -Lipolotio urea 5% F	1810043	1
Noweda	ALLERGIKA [®] -Lipolotio urea 5% F	2006020	1
	Aloe vera gel, 1:1	23000171002	1
	Aloe vera gel, 1:1	23001282002	1
	Aloe vera gel, 1:1	23000170001	1
	Aloe vera gel, 1:1	250426	1
Caelo	Aloe vera gel, 1:1	19255204	1
Caelo	Aloe vera gel, 1:1	20002878005	1
Caelo	Aloe vera gel, 1:1	18194304	3
Caelo	Aloe vera gel, 1:1	17289101	2
Caelo	Aloe vera gel, 1:1	19191401	7
Caelo	Aloe vera gel, 1:1	19069003	2
Caelo	Aloe vera gel, 1:1	19255202	1
Caelo	Aloe vera gel, 1:1	21001591003	2
Caelo	Aloe vera gel, 1:1	22001060003	1
Caelo	Aloe vera gel, 1:1	21002409001	1
Caelo	Aloe vera gel, 1:1	20000289003	7
Caelo	Aloe vera gel, 1:1	19069002	1
Caesar & Loretz GmbH	Aloe vera gel, 1:1	22001060004	1
Caesar & Loretz GmbH	Aloe vera gel, 1:1	22002254004	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Aloe vera gel, 1:1	22002254002	2
Caesar & Loretz Gm...	Aloe vera gel, 1:1	21002409002	7
Lamotte	Aloe vera gel, 1:1	19191403	1
Noweda	Aloe vera gel, 1:1	17289003	3
Phoenix	Aloe vera gel, 1:1	17134105	1
	Amciderm [®] Base cream	212181	1
Allmiral/Gehe	Amciderm [®] Base cream	418321	1
Almirall / Sanacorp	Amciderm [®] Base cream	48171	2
Almirall/Alliance	Amciderm [®] Base cream	650341	1
Almirall/Phönix	Amciderm [®] Base cream	538331	4
Almirall/Phönix	Amciderm [®] Base cream	822351	2
Almirall/Phönix	Amciderm [®] Base cream	12161	1
Fagron	Amciderm [®] Base cream	23102017	1
Dr. Wolff	Anefug [®] Simplex	136840	1
Argania Spinosa	Argan oil	A02148	1
Caelo	Argan oil	19098001	1
Caelo	Argan oil	18163408	1
Caelo	Argan oil	17198305	1
Caelo	Argan oil	18122701	2
Caelo	Argan oil	18163404	1
Caesar & Loretz GmbH	Argan oil	19116406	1
	Asche Basis [®] cream	220193	1
	Asche Basis [®] cream	31023A	34
	Asche Basis [®] cream	240022A	1
	Asche Basis [®] cream	2200027300	1
	Asche Basis [®] cream	33026A	17
	Asche Basis [®] cream	32025A	31
	Asche Basis [®] cream	32025a	1
	Asche Basis [®] cream	24021A	27
	Asche Basis [®] cream	23025A	1
	Asche Basis [®] cream	33027A	28
	Asche Basis [®] cream	2025A	1
	Asche Basis [®] cream	33027a	1
	Asche Basis [®] cream	34028A	8
	Asche Basis [®] cream	34029A	32
	Asche Basis [®] cream	34028a	1
	Asche Basis [®] cream	32024A	15
	Asche Basis [®] cream	42030A	25
	Asche Basis [®] cream	43031A	6
	Asche Basis [®] cream	23024	2
	Asche Basis [®] cream	42030a	1
	Asche Basis [®] cream	33026B	3
	Asche Basis [®] cream	24030A	1
	Asche Basis [®] cream	53033A	1
AHD	Asche Basis [®] cream	13009A	19
AHD	Asche Basis [®] cream	22019B	23
AHD/Chiesi	Asche Basis [®] cream	93444A	7
Alliance Healthcare	Asche Basis [®] cream	33240A	3
Anzag	Asche Basis [®] cream	23204A	2
Anzag/ Chiesi	Asche Basis [®] cream	42269A	1
Anzag/ Chiesi GmbH	Asche Basis [®] cream	42273A	3
Bombastus	Asche Basis [®] cream	290144	1
Caelo	Asche Basis [®] cream	53329A	11
Caelo	Asche Basis [®] cream	41265B	1
Caelo	Asche Basis [®] cream	52323a	1
Caelo	Asche Basis [®] cream	61341A	3
Caelo	Asche Basis [®] cream	61340A	2

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Supplier	Substance	Batch	Spectra
Caelo	Asche Basis [®] cream	61337A	3
Caelo	Asche Basis [®] cream	31226A	1
Caelo	Asche Basis [®] cream	20170829Ma4	1
Caelo	Asche Basis [®] cream	52322A	4
Caelo	Asche Basis [®] cream	4416I-03757	1
Caelo	Asche Basis [®] cream	83411A	12
Caelo	Asche Basis [®] cream	74391A	4
Caelo	Asche Basis [®] cream	83416A	11
Caesar & Loretz GmbH	Asche Basis [®] cream	20003818001	1
Chiese	Asche Basis [®] cream	41259A	2
Chiese	Asche Basis [®] cream	1449A	12
chiesi	Asche Basis [®] cream	7137A	1
Chiesi	Asche Basis [®] cream	24214A	3
Chiesi	Asche Basis [®] cream	24219A	1
Chiesi	Asche Basis [®] cream	24220A	2
Chiesi	Asche Basis [®] cream	23206A	1
Chiesi	Asche Basis [®] cream	14178A	1
Chiesi	Asche Basis [®] cream	32235A	2
Chiesi	Asche Basis [®] cream	31232A	2
Chiesi	Asche Basis [®] cream	24217A	1
Chiesi	Asche Basis [®] cream	33237A	3
Chiesi	Asche Basis [®] cream	33243A	1
Chiesi	Asche Basis [®] cream	34249A	2
Chiesi	Asche Basis [®] cream	34251A	3
Chiesi	Asche Basis [®] cream	34250A	2
Chiesi	Asche Basis [®] cream	41258A	3
Chiesi	Asche Basis [®] cream	41261A	2
Chiesi	Asche Basis [®] cream	42270A	1
Chiesi	Asche Basis [®] cream	30102014A	1
Chiesi	Asche Basis [®] cream	42272A	2
Chiesi	Asche Basis [®] cream	42271A	3
Chiesi	Asche Basis [®] cream	43280A	2
Chiesi	Asche Basis [®] cream	43278A	3
Chiesi	Asche Basis [®] cream	43262A	1
Chiesi	Asche Basis [®] cream	43279A	1
Chiesi	Asche Basis [®] cream	43287A	2
Chiesi	Asche Basis [®] cream	44288A	2
Chiesi	Asche Basis [®] cream	51294A	1
Chiesi	Asche Basis [®] cream	51296A	3
Chiesi	Asche Basis [®] cream	51305A	5
Chiesi	Asche Basis [®] cream	52307A	5
Chiesi	Asche Basis [®] cream	52323A	12
Chiesi	Asche Basis [®] cream	52315A	1
Chiesi	Asche Basis [®] cream	53326A	1
Chiesi	Asche Basis [®] cream	53330A	2
Chiesi	Asche Basis [®] cream	54332A	5
Chiesi	Asche Basis [®] cream	61338A	5
Chiesi	Asche Basis [®] cream	62343A	8
Chiesi	Asche Basis [®] cream	62344A	1
Chiesi	Asche Basis [®] cream	63347A	7
Chiesi	Asche Basis [®] cream	63354A	3
Chiesi	Asche Basis [®] cream	63355A	1
Chiesi	Asche Basis [®] cream	64357A	4
Chiesi	Asche Basis [®] cream	64360A	4
Chiesi	Asche Basis [®] cream	71367	1
Chiesi	Asche Basis [®] cream	64362A-20170704Ma4	1

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Supplier	Substance	Batch	Spectra
Chiesi	Asche Basis [®] cream	64364A	4
Chiesi	Asche Basis [®] cream	71370A	4
Chiesi	Asche Basis [®] cream	71372A	4
Chiesi	Asche Basis [®] cream	71373A	1
Chiesi	Asche Basis [®] cream	72379A	7
Chiesi	Asche Basis [®] cream	72378A	3
Chiesi	Asche Basis [®] cream	72382A	6
Chiesi	Asche Basis [®] cream	72384A	3
Chiesi	Asche Basis [®] cream	72383A	3
Chiesi	Asche Basis [®] cream	73389A	2
Chiesi	Asche Basis [®] cream	74390A	6
Chiesi	Asche Basis [®] cream	74392A	4
Chiesi	Asche Basis [®] cream	74397A	2
Chiesi	Asche Basis [®] cream	81404A	10
Chiesi	Asche Basis [®] cream	81400A	9
Chiesi	Asche Basis [®] cream	1(81404A)	1
Chiesi	Asche Basis [®] cream	72388A	1
Chiesi	Asche Basis [®] cream	81401A	10
Chiesi	Asche Basis [®] cream	81403A	2
Chiesi	Asche Basis [®] cream	82407A	12
Chiesi	Asche Basis [®] cream	82409A	8
Chiesi	Asche Basis [®] cream	83414A	6
Chiesi	Asche Basis [®] cream	84421A	11
Chiesi	Asche Basis [®] cream	84424A	13
Chiesi	Asche Basis [®] cream	91426A	17
Chiesi	Asche Basis [®] cream	84413A	1
Chiesi	Asche Basis [®] cream	91425A	17
Chiesi	Asche Basis [®] cream	91431A	10
Chiesi	Asche Basis [®] cream	92A36A	1
Chiesi	Asche Basis [®] cream	92432A	12
Chiesi	Asche Basis [®] cream	92433A	8
Chiesi	Asche Basis [®] cream	92442A	8
Chiesi	Asche Basis [®] cream	92441A	10
Chiesi	Asche Basis [®] cream	92439A	10
Chiesi	Asche Basis [®] cream	93446A	11
Chiesi	Asche Basis [®] cream	94448AI	1
Chiesi	Asche Basis [®] cream	94448AII	1
Chiesi	Asche Basis [®] cream	1450A	3
Chiesi	Asche Basis [®] cream	1454A	9
Chiesi	Asche Basis [®] cream	2457A	10
Chiesi	Asche Basis [®] cream	2460A	5
Chiesi	Asche Basis [®] cream	4004A	18
Chiesi	Asche Basis [®] cream	4003A	19
Chiesi	Asche Basis [®] cream	4006A	15
Chiesi	Asche Basis [®] cream	11001A	11
Chiesi	Asche Basis [®] cream	12005A	11
Chiesi	Asche Basis [®] cream	22019A	20
CHiesi	Asche Basis [®] cream	41264A	1
Chiesi / Gehe	Asche Basis [®] cream	33244A	3
Chiesi / Gehe	Asche Basis [®] cream	34252A	1
Chiesi / Gehe	Asche Basis [®] cream	41265A	1
Chiesi / Gehe	Asche Basis [®] cream	43281A	1
Chiesi / Gehe	Asche Basis [®] cream	51292A	1
Chiesi / Gehe	Asche Basis [®] cream	52314A	1
chiesi / Noweda	Asche Basis [®] cream	23213A	1
chiesi / Noweda	Asche Basis [®] cream	34250A	1

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Supplier	Substance	Batch	Spectra
Chiesi / Noweda	Asche Basis [®] cream	74393A	7
CHIESI / Noweda	Asche Basis [®] cream	51299A	3
Chiesi / Phoenix W...	Asche Basis [®] cream	53325A	1
Chiesi / Phönix	Asche Basis [®] cream	2458A	14
Chiesi / Sanacorp	Asche Basis [®] cream	24022A	33
chiesi /Jenne	Asche Basis [®] cream	31227a	1
Chiesi /jenne	Asche Basis [®] cream	84422A	9
Chiesi GmbH	Asche Basis [®] cream	52319A	1
Chiesi GmbH	Asche Basis [®] cream	52309A	4
Chiesi GmbH	Asche Basis [®] cream	61335A	2
Chiesi GmbH	Asche Basis [®] cream	64359A	3
Chiesi GmbH	Asche Basis [®] cream	64363A	6
Chiesi GmbH	Asche Basis [®] cream	64365A	3
Chiesi GmbH	Asche Basis [®] cream	92440A	6
Chiesi GmbH	Asche Basis [®] cream	93447A	7
Chiesi GmbH	Asche Basis [®] cream	2456A	22
Chiesi GmbH	Asche Basis [®] cream	12007A	14
Chiesi GmbH	Asche Basis [®] cream	14012A	12
Chiesi GmbH	Asche Basis [®] cream	24021B	22
Chiesi GmbH / Anzag	Asche Basis [®] cream	22196A	1
Chiesi GmbH / Anzag	Asche Basis [®] cream	31230A	1
Chiesi GmbH / Anzag	Asche Basis [®] cream	31229A	3
Chiesi GmbH / Anzag	Asche Basis [®] cream	31231A	2
Chiesi GmbH / Anzag	Asche Basis [®] cream	41260A	4
Chiesi GmbH / Anzag	Asche Basis [®] cream	42268A	2
Chiesi GmbH / Gehe	Asche Basis [®] cream	94448a	1
Chiesi GmbH/ Phönix	Asche Basis [®] cream	11003A	24
Chiesi GmbH/AHD	Asche Basis [®] cream	84420A	8
Chiesi GmbH/Gehe	Asche Basis [®] cream	61341A, 20161215Ma2	1
Chiesi GmbH/Gehe	Asche Basis [®] cream	61342A, 20161215Ma3	1
Chiesi GmbH/Noweda	Asche Basis [®] cream	12006A	13
Chiesi GmbH/Noweda	Asche Basis [®] cream	14017A	25
Chiesi GmbH/Phoenix	Asche Basis [®] cream	14015A	16
Sino Phyto	Asche Basis [®] cream	74394A	9
Chiesi Sanacorp	Asche Basis [®] cream	120005A	1
Chiesi Sanacorp	Asche Basis [®] cream	13010A	13
chiesi-	Asche Basis [®] cream	71372A20171127Ma13	1
chiesi-	Asche Basis [®] cream	72376A-20180830Ma8	1
Chiesi-Fa.Gehe	Asche Basis [®] cream	81401A-A20190115Ma11	1
Chiesi-Fa.Gehe 19.6.18	Asche Basis [®] cream	74391A-20180830Ma7	1
Chiesi,Fa.Gehe	Asche Basis [®] cream	52314A, 20160225/1	1
Chiesi,Gehe	Asche Basis [®] cream	52320A, 20160504Ma6	1
Chiesi/	Asche Basis [®] cream	41266A	1
Chiesi/ Noweda	Asche Basis [®] cream	64358A	8
Chiesi/ Fiebig	Asche Basis [®] cream	63356A	1
Chiesi/ Fiebig	Asche Basis [®] cream	72376A	3
Chiesi/ Now	Asche Basis [®] cream	43283A	3
Chiesi/ Noweda	Asche Basis [®] cream	51294a	1
Chiesi/ Noweda	Asche Basis [®] cream	170420AB/63353A	1
Chiesi/ Noweda	Asche Basis [®] cream	170601ABC/64357A	1
Chiesi/ Noweda	Asche Basis [®] cream	170628ABC/64362A	1
Chiesi/ Noweda	Asche Basis [®] cream	170706ABC/64361A	1
Chiesi/ Noweda	Asche Basis [®] cream	170816AB/64364A	1
Chiesi/ Noweda	Asche Basis [®] cream	170927AB/71370A	1
Chiesi/ Noweda	Asche Basis [®] cream	171025AB/71371A	1
Chiesi/ Noweda	Asche Basis [®] cream	71371A	2

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Supplier	Substance	Batch	Spectra
Chiesi/ Noweda	Asche Basis [®] cream	171215ABC/72376A	1
Chiesi/ Noweda	Asche Basis [®] cream	171228ABC/72376A	1
Chiesi/ Noweda	Asche Basis [®] cream	180219AB/72379A	1
Chiesi/ phoenix	Asche Basis [®] cream	33239A	3
Chiesi/ Phönix	Asche Basis [®] cream	4002A	15
Chiesi/ Sanacorp	Asche Basis [®] cream	1451A	10
Chiesi/ Sanacorp	Asche Basis [®] cream	12004A	17
Chiesi/AEP	Asche Basis [®] cream	82405A	10
Chiesi/AHD	Asche Basis [®] cream	31222A	3
Chiesi/AHD	Asche Basis [®] cream	31223A	1
Chiesi/AHD	Asche Basis [®] cream	31228A	3
Chiesi/AHD	Asche Basis [®] cream	32234A	1
Chiesi/AHD	Asche Basis [®] cream	33238A	2
Chiesi/AHD	Asche Basis [®] cream	33242A	1
Chiesi/Alliance He...	Asche Basis [®] cream	44290A	5
Chiesi/Anzag	Asche Basis [®] cream	24221A	7
Chiesi/Anzag	Asche Basis [®] cream	43282A	2
Chiesi/Anzag	Asche Basis [®] cream	51295A	1
Chiesi/Anzag	Asche Basis [®] cream	53327A	2
Chiesi/Anzag	Asche Basis [®] cream	2(91431A)	1
Chiesi/Anzag	Asche Basis [®] cream	221109(21018A)	1
Chiesi/Ebert	Asche Basis [®] cream	31224A	4
Chiesi/Fiebig	Asche Basis [®] cream	733864A	1
chiesi/gehe	Asche Basis [®] cream	32236A	3
Chiesi/Gehe	Asche Basis [®] cream	24218A	2
Chiesi/Gehe	Asche Basis [®] cream	32233A	7
Chiesi/Gehe	Asche Basis [®] cream	34248A	2
Chiesi/Gehe	Asche Basis [®] cream	34253A	1
Chiesi/Gehe	Asche Basis [®] cream	41262A	1
Chiesi/Gehe	Asche Basis [®] cream	51300A	9
Chiesi/Gehe	Asche Basis [®] cream	51301A	1
Chiesi/Gehe	Asche Basis [®] cream	71369A	2
Chiesi/Gehe	Asche Basis [®] cream	72377A	3
Chiesi/Gehe	Asche Basis [®] cream	82408A	5
Chiesi/Gehe	Asche Basis [®] cream	83413A	16
Chiesi/Gehe	Asche Basis [®] cream	941426A	1
Chiesi/Gehe	Asche Basis [®] cream	963444A	1
Chiesi/Gehe	Asche Basis [®] cream	93445A	7
Chiesi/Gehe	Asche Basis [®] cream	21018A	21
Chiesi/Gehe	Asche Basis [®] cream	22020A	36
chiesi/hageda	Asche Basis [®] cream	63347a	1
Chiesi/Hageda	Asche Basis [®] cream	13008A	14
Chiesi/Jenne	Asche Basis [®] cream	72381A	3
Chiesi/Jenne	Asche Basis [®] cream	14013A	10
Chiesi/Jenne	Asche Basis [®] cream	14014A	14
Chiesi/Jenne	Asche Basis [®] cream	14016A	11
Chiesi/Kehr	Asche Basis [®] cream	20008410/0	1
Chiesi/Krieger	Asche Basis [®] cream	74396A	6
Chiesi/Krieger	Asche Basis [®] cream	81402A	13
Chiesi/Krieger	Asche Basis [®] cream	91427A	8
Chiesi/Krieger	Asche Basis [®] cream	92442A/	1
Chiesi/Krieger	Asche Basis [®] cream	1452A	6
Chiesi/Noweda	Asche Basis [®] cream	42275A	2
Chiesi/Noweda	Asche Basis [®] cream	52306A	7
Chiesi/Noweda	Asche Basis [®] cream	52318A	3
Chiesi/Noweda	Asche Basis [®] cream	52318a	1

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Supplier	Substance	Batch	Spectra
Chiesi/Noweda	Asche Basis [®] cream	6234A	1
Chiesi/Noweda	Asche Basis [®] cream	170421AB/63353A	1
Chiesi/Noweda	Asche Basis [®] cream	171211AB/72376A	1
Chiesi/Noweda	Asche Basis [®] cream	180112ABC/72378A	1
Chiesi/Noweda	Asche Basis [®] cream	180322AB/72382A	1
Chiesi/Noweda	Asche Basis [®] cream	844194	1
Chiesi/Noweda	Asche Basis [®] cream	92434A	15
Chiesi/Noweda	Asche Basis [®] cream	13011A	10
chiesi/Phoen	Asche Basis [®] cream	73388A	10
Chiesi/phoenix	Asche Basis [®] cream	92436A	19
Chiesi/Phoenix	Asche Basis [®] cream	24215A	1
Chiesi/Phoenix	Asche Basis [®] cream	31227A	6
Chiesi/Phoenix	Asche Basis [®] cream	31225A	2
Chiesi/Phoenix	Asche Basis [®] cream	53331A	8
Chiesi/Phoenix	Asche Basis [®] cream	71368A	4
Chiesi/Phoenix	Asche Basis [®] cream	93443A	17
Chiesi/Phönix	Asche Basis [®] cream	61334A	2
Chiesi/Phönix	Asche Basis [®] cream	72375A	6
Chiesi/Phönix	Asche Basis [®] cream	72385A	4
Chiesi/Phönix	Asche Basis [®] cream	83412A	11
Chiesi/Phönix	Asche Basis [®] cream	84419A	14
Chiesi/Phönix	Asche Basis [®] cream	91429A	11
Chiesi/Phönix	Asche Basis [®] cream	92437A	19
Chiesi/Phönix	Asche Basis [®] cream	92438A	4
Chiesi/Phönix	Asche Basis [®] cream	1455A	12
Chiesi/Phönix	Asche Basis [®] cream	2459A	8
Chiesi/Phönix	Asche Basis [®] cream	11002A	16
Chiesi/Phönix WE:2...	Asche Basis [®] cream	64362A	2
chiesi/sanacorp	Asche Basis [®] cream	1453A	11
Chiesi/sanacorp	Asche Basis [®] cream	4005A	10
Chiesi/Sanacorp	Asche Basis [®] cream	84423A	6
Chiesi/Sanacorp WE...	Asche Basis [®] cream	52317A	1
Spangropharm	Asche Basis [®] cream	82093A	1
Chiesie GmbH/Phönix	Asche Basis [®] cream	83415A	3
Chiesi	Asche Basis [®] cream	52310A	5
Chisi	Asche Basis [®] cream	23203A	1
Dr.Wolff	Asche Basis [®] cream	63348A, 20170427Ma3	1
Euro OTC	Asche Basis [®] cream	3229A	1
Euro OTC	Asche Basis [®] cream	3616Q-03757	1
Fa.Chiesi/Gehe	Asche Basis [®] cream	91430A	12
Fa.Gehe	Asche Basis [®] cream	20160727Ma4	1
Fagron	Asche Basis [®] cream	63353A	3
Fiebig	Asche Basis [®] cream	91428A	7
Galaderma/Krieger	Asche Basis [®] cream	17370A	1
Gehe	Asche Basis [®] cream	52321A	1
GEHE	Asche Basis [®] cream	73387A	8
GEHE	Asche Basis [®] cream	81399A	11
Gehe-Chiesi	Asche Basis [®] cream	52308A	5
Hedinger	Asche Basis [®] cream	74398A	7
Kremer	Asche Basis [®] cream	71367A	8
Lamotte / Gehe	Asche Basis [®] cream	34247A	4
Lamotte/phoe	Asche Basis [®] cream	2916I-03757	1
Lamotte/phoe	Asche Basis [®] cream	2616J-03757	1
Noweda	Asche Basis [®] cream	84417A	16
Noweda	Asche Basis [®] cream	84418A	19
Noweda	Asche Basis [®] cream	92435A	9

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Supplier	Substance	Batch	Spectra
Noweda	Asche Basis [®] cream	3461A	12
Noweda/Chiesi	Asche Basis [®] cream	73386A	14
Noweda/Chiesi	Asche Basis [®] cream	94448A	6
phoenix	Asche Basis [®] cream	72380A	9
phoenix	Asche Basis [®] cream	82410A	12
Phoenix	Asche Basis [®] cream	5331A	1
Phoenix	Asche Basis [®] cream	71374A	6
Phoenix/Chiesi	Asche Basis [®] cream	33246A	4
Phoenix/Chiesi	Asche Basis [®] cream	61333A	1
Phönix	Asche Basis [®] cream	322344	1
Phönix/Chiesi 07.12.20	Asche Basis [®] cream	24564A	1
PhönixWE:3.02.2017...	Asche Basis [®] cream	63350A	3
Sanacorp / Wolff	Asche Basis [®] cream	82A05A	1
Sanacorp WE 20.02...	Asche Basis [®] cream	63351A	4
Sanacorp/langenhagen	Asche Basis [®] cream	43032A	20
THC/ Phönix	Asche Basis [®] cream	129880	1
Pharma...			
WE: Phoenix 23.09...	Asche Basis [®] cream	61339A	1
WE:Phönix28.07.201...	Asche Basis [®] cream	61336A	1
Wolff/ Sanacorp	Asche Basis [®] cream	810201	1
Wolff/Gehe	Asche Basis [®] cream	71366A	1
Wolff/Gehe	Asche Basis [®] cream	64365A-20171106Ma10	1
	Asche Basis [®] fat ointment	24009A	1
	Asche Basis [®] fat ointment	33011A	1
	Asche Basis [®] fat ointment	41013A	3
Chiese	Asche Basis [®] fat ointment	33016A	1
Chiese	Asche Basis [®] fat ointment	63023A	2
Chiesi	Asche Basis [®] fat ointment	81026A	1
Chiesi	Asche Basis [®] fat ointment	82027A	4
Chiesi	Asche Basis [®] fat ointment	84028A	2
CHiesi	Asche Basis [®] fat ointment	41018A	3
Chiesi GmbH	Asche Basis [®] fat ointment	14007A	1
Chiesi GmbH/Phönix	Asche Basis [®] fat ointment	93029A	3
Chiesi/ Sanacorp	Asche Basis [®] fat ointment	2001A	1
Chiesi/Gehe	Asche Basis [®] fat ointment	51020A	2
Chiesi/Gehe	Asche Basis [®] fat ointment	41017A	1
Chiesi/Jenne	Asche Basis [®] fat ointment	24010A	1
Chiesi/Phönix	Asche Basis [®] fat ointment	73025A	4
	Asche Basis [®] lotion	23009A	7
	Asche Basis [®] lotion	23009a	1
	Asche Basis [®] lotion	31010A	9
	Asche Basis [®] lotion	31011A	13
	Asche Basis [®] lotion	33012A	19
	Asche Basis [®] lotion	33013A	14
	Asche Basis [®] lotion	41014A	10
	Asche Basis [®] lotion	41015A	9
	Asche Basis [®] lotion	44016A	3
Aenov Groupe	Asche Basis [®] lotion	40000200790	1
Aenova	Asche Basis [®] lotion	93102A	5
Alliance Healthcare	Asche Basis [®] lotion	82094A	3
Alliance Healthcare	Asche Basis [®] lotion	91098A	7
Alliance Healthcare	Asche Basis [®] lotion	91099A	3
Caelo	Asche Basis [®] lotion	33055A	3
Caelo	Asche Basis [®] lotion	53073A	6
Caelo	Asche Basis [®] lotion	73089A	3
Chiese	Asche Basis [®] lotion	41060A	1

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Supplier	Substance	Batch	Spectra
Chiesi	Asche Basis [®] lotion	333056A	2
Chiesi	Asche Basis [®] lotion	42062A	2
Chiesi	Asche Basis [®] lotion	43065A	2
Chiesi	Asche Basis [®] lotion	42063A	1
Chiesi	Asche Basis [®] lotion	53074A	5
Chiesi	Asche Basis [®] lotion	73085A	2
Chiesi	Asche Basis [®] lotion	46082A	1
Chiesi	Asche Basis [®] lotion	73087A	1
Chiesi	Asche Basis [®] lotion	75085A	1
Chiesi	Asche Basis [®] lotion	73088A	5
Chiesi	Asche Basis [®] lotion	73088a	1
Chiesi	Asche Basis [®] lotion	84096A	1
Chiesi	Asche Basis [®] lotion	92101A	6
Chiesi	Asche Basis [®] lotion	1107A	8
Chiesi	Asche Basis [®] lotion	11003A	5
Chiesi	Asche Basis [®] lotion	2100A	1
Chiesi	Asche Basis [®] lotion	21007A	6
Chiesi / Noweda / ...	Asche Basis [®] lotion	82093A	1
Chiesi GmbH	Asche Basis [®] lotion	53071A	6
Chiesi GmbH	Asche Basis [®] lotion	61076A	3
Chiesi GmbH	Asche Basis [®] lotion	63079A	2
Chiesi GmbH	Asche Basis [®] lotion	73087A	5
Chiesi GmbH	Asche Basis [®] lotion	2001A	7
Chiesi GmbH	Asche Basis [®] lotion	13006A	15
Chiesi GmbH / Phönix	Asche Basis [®] lotion	51067A	2
Chiesi GmbH/Gehe	Asche Basis [®] lotion	53072A	6
Chiesi-Fa.Gehe	Asche Basis [®] lotion	64082A-20180112Ma3	1
Chiesi-Fa.Gehe	Asche Basis [®] lotion	73086A-20180206Ma8	1
Chiesi-Fa.Gehe	Asche Basis [®] lotion	73087A-20180206Ma9	1
Chiesi-Fa.Gehe	Asche Basis [®] lotion	82093A-A20181115Ma1	1
Chiesi-Fa.Gehe 19.7.18	Asche Basis [®] lotion	74090A-20180830Ma10	1
Chiesi/ Fiebig	Asche Basis [®] lotion	63980A	6
Chiesi/ Phoenix/ 3...	Asche Basis [®] lotion	1108A	3
Chiesi/ Phoenix/ 11...	Asche Basis [®] lotion	941044	1
Chiesi/ Phönix	Asche Basis [®] lotion	43066A	3
Chiesi/AHD	Asche Basis [®] lotion	24049A	2
Chiesi/Alliance	Asche Basis [®] lotion	63981A	4
Chiesi/Alliance	Asche Basis [®] lotion	11004A	4
Chiesi/Anzag	Asche Basis [®] lotion	41059A	3
Chiesi/E+J	Asche Basis [®] lotion	64082A	11
Chiesi/Fa.Gehe	Asche Basis [®] lotion	53075A	7
Chiesi/Fiebig	Asche Basis [®] lotion	73086A	4
chiesi/gehe	Asche Basis [®] lotion	33056A	2
chiesi/gehe	Asche Basis [®] lotion	34058A	1
Chiesi/Gehe	Asche Basis [®] lotion	23047A	1
Chiesi/Gehe	Asche Basis [®] lotion	2002A	4
Chiesi/Noweda	Asche Basis [®] lotion	61077A	2
Chiesi/Noweda	Asche Basis [®] lotion	13005A	8
Chiesi/phönix	Asche Basis [®] lotion	82092A	15
Chiesi/Phönix	Asche Basis [®] lotion	84095A	6
Chiesi/Phönix	Asche Basis [®] lotion	94106A	16
Chiesie/Anzag	Asche Basis [®] lotion	32054A	4
Devesa	Asche Basis [®] lotion	63078A	5
Fa. Chiesi/Gehe	Asche Basis [®] lotion	92100A	12
Fa. Chiesi/Noweda	Asche Basis [®] lotion	91097A	16
Fa.Chiesi/Noweda	Asche Basis [®] lotion	94104A	8

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Supplier	Substance	Batch	Spectra
Fa.Chiesi/Noweda	Asche Basis [®] lotion	94105A	9
Fa.Gehe	Asche Basis [®] lotion	20160727Ma5	1
Fiebig/Chiesi	Asche Basis [®] lotion	71083A	3
Fiebig/Chiesi	Asche Basis [®] lotion	71084A	3
Gehe	Asche Basis [®] lotion	82082A	1
Gehe Chiesi	Asche Basis [®] lotion	53075A-20160615Ma5	1
Gehe20.10.15	Asche Basis [®] lotion	52070A	2
Noweda	Asche Basis [®] lotion	93103A	10
Bombastus	Asche Basis [®] lotion	74091A	2
Caelo	Asche Basis [®] lotion	64082a	1
Phoenix	Asche Basis [®] lotion	52069A	2
Sanacorp	Asche Basis [®] lotion	84096	1
Sanacorp	Asche Basis [®] lotion	23008A	8
	Asche Basis [®] ointment	310012A	1
	Asche Basis [®] ointment	31012A	9
	Asche Basis [®] ointment	33013a	1
	Asche Basis [®] ointment	33014A	5
	Asche Basis [®] ointment	34016A	4
	Asche Basis [®] ointment	34017A	6
	Asche Basis [®] ointment	41018A	4
	Asche Basis [®] ointment	42020A	4
	Asche Basis [®] ointment	42019A	2
Alliance	Asche Basis [®] ointment	33015A	6
Anzag/Ichtyol-Gese...	Asche Basis [®] ointment	23043A	1
Caelo	Asche Basis [®] ointment	81708A	1
chiesi	Asche Basis [®] ointment	42055A	1
chiesi	Asche Basis [®] ointment	44057A	1
Chiesi	Asche Basis [®] ointment	34051A	1
Chiesi	Asche Basis [®] ointment	41052A	1
Chiesi	Asche Basis [®] ointment	41054A	4
Chiesi	Asche Basis [®] ointment	51060A	1
Chiesi	Asche Basis [®] ointment	52063A	7
Chiesi	Asche Basis [®] ointment	94087A	6
Chiesi	Asche Basis [®] ointment	14006A	7
Chiesi	Asche Basis [®] ointment	22010A	10
Chiesi	Asche Basis [®] ointment	24011A	3
Chiesi / Gehe	Asche Basis [®] ointment	33050A	1
Chiesi / Phönix	Asche Basis [®] ointment	92084A	10
Chiesi / Phönix	Asche Basis [®] ointment	92087A	1
chiesi /Gehe	Asche Basis [®] ointment	73075A	5
Chiesi /Jenne	Asche Basis [®] ointment	92437A	1
Chiesi GmbH	Asche Basis [®] ointment	21039A	1
Chiesi GmbH	Asche Basis [®] ointment	52062A	5
Chiesi GmbH	Asche Basis [®] ointment	52064A	5
Chiesi GmbH	Asche Basis [®] ointment	53065A	6
Chiesi GmbH	Asche Basis [®] ointment	63069A	4
Chiesi GmbH	Asche Basis [®] ointment	71071A	1
Chiesi GmbH / Sanacorp	Asche Basis [®] ointment	92034A	1
Chiesi GmbH / Sanacorp	Asche Basis [®] ointment	21008A	8
Chiesi GmbH/ Gehe	Asche Basis [®] ointment	13005A	12
Chiesi GmbH/ Gehe	Asche Basis [®] ointment	13004A	3
Chiesi GmbH/GEHE	Asche Basis [®] ointment	22009A	9
Chiesi GmbH/Phoenix	Asche Basis [®] ointment	91082A	10
CHIESI/ NOWEDA	Asche Basis [®] ointment	51060A	3
Chiesi/ sanacorp	Asche Basis [®] ointment	92086A	8
Chiesi/AHD	Asche Basis [®] ointment	31045A	4

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Supplier	Substance	Batch	Spectra
Chiesi/AHD	Asche Basis [®] ointment	33049A	3
Chiesi/Anzag	Asche Basis [®] ointment	1 (92084A)	1
Chiesi/Anzag	Asche Basis [®] ointment	11002A	12
Chiesi/Gehe	Asche Basis [®] ointment	42056A	1
Chiesi/Gehe	Asche Basis [®] ointment	83079A	9
Chiesi/Gehe	Asche Basis [®] ointment	33013A	4
Chiesi/Jenne	Asche Basis [®] ointment	73076A	2
Chiesi/Jenne	Asche Basis [®] ointment	74077A	3
Chiesi/Jenne	Asche Basis [®] ointment	925084A	1
Chiesi/Jenne	Asche Basis [®] ointment	6.2022	1
Chiesi/Jenne	Asche Basis [®] ointment	2001A	4
Chiesi/Krieger	Asche Basis [®] ointment	61066A	3
Chiesi/Noweda	Asche Basis [®] ointment	71072A	7
Chiesi/Noweda	Asche Basis [®] ointment	12003A	9
Chiesi/Phoenix	Asche Basis [®] ointment	23042A	1
Chiesi/Phoenix	Asche Basis [®] ointment	2089A	11
Chiesi/Phoenix	Asche Basis [®] ointment	3090A	9
Chiesi/Phoenix	Asche Basis [®] ointment	21007A	17
Chiesi/Phönix	Asche Basis [®] ointment	51059A	1
Chiesi/Phönix	Asche Basis [®] ointment	71073A	4
Chiesi/Phönix	Asche Basis [®] ointment	72074A	3
Chiesi/Phönix	Asche Basis [®] ointment	81078A	1
Chiesi/Phönix	Asche Basis [®] ointment	84081A	10
Chiesi/Sanacorp	Asche Basis [®] ointment	41053A	1
Chiesi/Sanacorp	Asche Basis [®] ointment	83080A	10
Chiesi/Sanacorp	Asche Basis [®] ointment	92085A	6
Gehe	Asche Basis [®] ointment	17I21-B01	1
Caelo	Asche Basis [®] ointment	63068A	5
Caelo	Asche Basis [®] ointment	61067A	5
Noweda	Asche Basis [®] ointment	2088A	10
Phönix	Asche Basis [®] ointment	31047A	3
Phönix/ Chiesi	Asche Basis [®] ointment	92083A	17
Sanacorp WE 29.04...	Asche Basis [®] ointment	63070A	4
Wolff/AHD	Asche Basis [®] ointment	32048A	3

B

Supplier	Substance	Batch	Spectra
Taoasis	Balm Bio Nature	151210-5337	12
	Base cream DVL-P	L098E23	2
	Base cream DVL-P	L071F24	1
	Base cream DVL-P	L027S24	1
	Base cream DVL-P	L034B25	1
/Sanacorp	Base cream Taoasis	180718-7100	5
Bombastus	Base cream Taoasis	180307	1
Caelo	Base cream Taoasis	20001006001	1
Fagron	Base cream Taoasis	20B10-T13-075420	1
Caelo	Base cream Taoasis	2010280197	1
Phoenix/bomb	Base cream Taoasis	210716-1124	6
taoasis	Base cream Taoasis	180307-8030	1
Taoasis	Base cream Taoasis	150219-4350	1
Taoasis	Base cream Taoasis	150326-5079	1
Taoasis	Base cream Taoasis	160201-6027	1
Taoasis	Base cream Taoasis	161124-6322	1
Taoasis	Base cream Taoasis	170110-6322	2
Taoasis	Base cream Taoasis	181204-8333	1
Taoasis	Base cream Taoasis	190920-9182A	1
Taoasis	Base cream Taoasis	200303-9344	2
Taoasis	Base cream Taoasis	200708-0079	3

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Supplier	Substance	Batch	Spectra
Taoasis	Base cream Taoasis	SAP2638-2019	2
Taoasis	Base cream Taoasis	SAP2792-2216	5
Taoasis	Base cream Taoasis	SAP3344-3115	4
Taoasis	Base cream Taoasis	SAP3466-3139	3
Taoasis	Base cream Taoasis	SAP3467-3142	11
Taoasis	Base cream Taoasis	SAP4104-4030	3
Taoasis GmbH	Base cream Taoasis	190206-9030	1
Taoasis GmbH	Base cream Taoasis	1911259290	1
Taoasis GmbH	Base cream Taoasis	191125-9290	1
Taoasis GmbH	Base cream Taoasis	201028-0197	1
Taoasis GmbH	Base cream Taoasis	14848DEP02	1
Taoasis GmbH/ Taoasis	Base cream Taoasis	190916-9182	1
TAOASIS/Hageda	Base cream Taoasis	SAP2637-1252	1
Taoasis/Sanacorp	Base cream Taoasis	170317-7031	4
Taoasis/Sanacorp	Base cream Taoasis	170517-7100	3
Taoasis/Sanacorp	Base cream Taoasis	1807187100	1
Taoasis/Sanacorp	Base cream Taoasis	171127-7290	12
Taoasis/Sanacorp	Base cream Taoasis	180924-8114	3
Taoasis/Sanacorp	Base cream Taoasis	180515-8030	1
Taoasis/Sanacorp	Base cream Taoasis	SAP2728-2019	2
Taoasis/Taoasis	Base cream Taoasis	210309-0343	1
Taoasis	Base cream Taoasis	18384	1
Fischer	Bepanthen® solution	6317104	1
Caelo	Bepanthen® solution	KV02S8P	1
Liechtenstein	Bepanthen® solution	2300380R	1
Bayer	Bepanthen® Wund- und Heilsalbe	GP01AUE	1
Bayer	Bepanthen® Wund- und Heilsalbe	GP01R60	1
Bayer/Phönix	Bepanthen® Wund- und Heilsalbe	G001XHE	1
Bombastus	Bepanthen® Wund- und Heilsalbe	GP01-DR9	1

C

Supplier	Substance	Batch	Spectra
Anzag	Capsaicin liquid extract 3%	120503801	1
Euro OTC	Capsaicin liquid extract 3%	6061204	1
Euro OTC	Capsaicin liquid extract 3%	12111205	1
Euro OTC	Capsaicin liquid extract 3%	1201010-01	1
Euro OTC	Capsaicin liquid extract 3%	1205038-01	2
EUro/AHD	Capsaicin liquid extract 3%	1205038-02	1
Caelo	Common wormwood oil	79363	1

D

Supplier	Substance	Batch	Spectra
Caelo	Dermatest base ointment	40622	7
Galderma	Dermatest base ointment	200419	3
Noweda	Dermatest base ointment	301026	1
P&M	Dermatest base ointment	241115	1
P&M Cosmetics	Dermatest base ointment	210915	1
p&M Cosmetics GmbH	Dermatest base ointment	270623	5
P&M Cosmetics/Alliance	Dermatest base ointment	160820	1
P&M Cosmetics/Alli...	Dermatest base ointment	152241	1
P&M Cosmetics/Anzag	Dermatest base ointment	122631	1
P&M Cosmetics/Noweda	Dermatest base ointment	301124	5
P&M/Alliance	Dermatest base ointment	121217	3
P&M/Alliance	Dermatest base ointment	190317	1
P&M/Alliance	Dermatest base ointment	260820	7
Pm Cosmetica/Gehe	Dermatest base ointment	280821	9

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Supplier	Substance	Batch	Spectra
Sanacorp	Dermatest base ointment	70615	1
	Dermatop [®] base cream	3F118A	1
	Dermatop [®] base cream	G48830	1
	Dermatop [®] base cream	H07540	1
	Dermatop [®] base cream	H26330	1
	Dermatop [®] base cream	H26590	1
	Dermatop [®] base cream	H28170	2
	Dermatop [®] base cream	H48860	1
	Dermatop [®] base cream	H29560	2
alliance	Dermatop [®] base cream	2F116A	1
Euro OTC	Dermatop [®] base cream	8F077A	1
Fidia	Dermatop [®] base cream	2F110A	1
FIDIA	Dermatop [®] base cream	2F112A	1
Klindwort Apotheke...	Dermatop [®] base cream	8F075A	2
Noweda	Dermatop [®] base cream	2F117A	1
Phönix	Dermatop [®] base cream	7F072A	2
Phönix	Dermatop [®] base cream	8F076A	2
Phönix/Sanofi	Dermatop [®] base cream	9F087A	1
Phönix/Sanofi	Dermatop [®] base cream	0F095A	1
Sanofi	Dermatop [®] base cream	0F092A	1
Sanofi	Dermatop [®] base cream	1F107A	3
Sanofi / Gehe	Dermatop [®] base cream	4F046A	4
Sanofi / Phönix	Dermatop [®] base cream	8F082A	2
Sanofi / Phönix	Dermatop [®] base cream	9F087A	3
Sanofi / Phönix	Dermatop [®] base cream	9F090A	3
Sanofi / Phönix	Dermatop [®] base cream	94090A	1
Sanofi / Phönix	Dermatop [®] base cream	F092A	3
Sanofi / Phönix	Dermatop [®] base cream	0F094A	1
Sanofi / Phönix	Dermatop [®] base cream	F92A	1
Sanofi / Phönix	Dermatop [®] base cream	f092A	1
Sanofi / Phönix	Dermatop [®] base cream	0F096A	2
Sanofi / Phönix	Dermatop [®] base cream	F098B	1
Sanofi /Noweda	Dermatop [®] base cream	F098A	1
Sanofi-Aventis Deu...	Dermatop [®] base cream	F096A	4
Sanofi-Aventis/Phönix	Dermatop [®] base cream	6F065A	1
Sanofi/AllianceHea...	Dermatop [®] base cream	F091A	2
Sanofi/Anzag	Dermatop [®] base cream	5F051A	3
Sanofi/Gehe	Dermatop [®] base cream	4F050A	1
Sanofi/Noweda	Dermatop [®] base cream	5F056A	2
Sanofi/Phoenix	Dermatop [®] base cream	F099A	2
Sanofi/Phoenix	Dermatop [®] base cream	1F103A	1
Sanofi/Phönix	Dermatop [®] base cream	7F071A	2
Sanofi/Phönix	Dermatop [®] base cream	7F073A	2
Sanofi/Phönix	Dermatop [®] base cream	7F069A	1
Sanofi/Phönix	Dermatop [®] base cream	8F074A	3
Sanofi/Phönix	Dermatop [®] base cream	8F078A	2
Sanofi/Phönix	Dermatop [®] base cream	8F079A	1
Sanofi/Phönix	Dermatop [®] base cream	8F080A	3
Sanofi/Phönix	Dermatop [®] base cream	8F081A	2
Sanofi/Phönix	Dermatop [®] base cream	8F084A	7
Sanofi/Phönix	Dermatop [®] base cream	8F083A	3
Sanofi/Phönix	Dermatop [®] base cream	8F082B	1
Sanofi/Phönix	Dermatop [®] base cream	9F086A	1
Sanofi/Phönix	Dermatop [®] base cream	9F089A	2
	Dermatop [®] base ointment	3F167A	5
	Dermatop [®] base ointment	H26020	2

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Supplier	Substance	Batch	Spectra
	Dermatop [®] base ointment	H50010	1
Caelo	Dermatop [®] base ointment	8F125A	6
Caelo	Dermatop [®] base ointment	5F080A	1
Caelo	Dermatop [®] base ointment	7F107A	1
Fidia / Noweda	Dermatop [®] base ointment	2F158A	1
Galderma/Noweda	Dermatop [®] base ointment	8F123A	2
Noweda	Dermatop [®] base ointment	2F162A	1
Phönix	Dermatop [®] base ointment	7F108B	1
Sanacorp/Sanofi WE...	Dermatop [®] base ointment	5F086A	1
sanofi	Dermatop [®] base ointment	F140A	6
sanofi	Dermatop [®] base ointment	0F144A	5
Sanofi	Dermatop [®] base ointment	4F073A	1
Sanofi	Dermatop [®] base ointment	5F082A	1
Sanofi	Dermatop [®] base ointment	6F095A	1
Sanofi	Dermatop [®] base ointment	7F106A	1
Sanofi	Dermatop [®] base ointment	8F124A	5
Sanofi	Dermatop [®] base ointment	8F127A	1
Sanofi	Dermatop [®] base ointment	9F127A	2
Sanofi	Dermatop [®] base ointment	9F128A	5
Sanofi	Dermatop [®] base ointment	9F178A	1
Sanofi	Dermatop [®] base ointment	9F130A	2
Sanofi	Dermatop [®] base ointment	9F131A	3
Sanofi	Dermatop [®] base ointment	9F134A	8
Sanofi	Dermatop [®] base ointment	9F129A	4
Sanofi	Dermatop [®] base ointment	F138A	5
Sanofi - Noweda	Dermatop [®] base ointment	5F089A	1
Sanofi / Alliance ...	Dermatop [®] base ointment	6F094A	2
Sanofi / Alliance ...	Dermatop [®] base ointment	8F118A	1
Sanofi / Phönix	Dermatop [®] base ointment	F136A	3
Sanofi /Noweda	Dermatop [®] base ointment	0F135A	3
Sanofi /Noweda	Dermatop [®] base ointment	0F137A	1
Sanofi /Noweda	Dermatop [®] base ointment	F143A	2
Sanofi /Noweda	Dermatop [®] base ointment	F142A	2
Sanofi /Noweda	Dermatop [®] base ointment	1F145A	2
Sanofi Aventis / S...	Dermatop [®] base ointment	F141A	1
Sanofi-Aventis	Dermatop [®] base ointment	7F103A	1
Sanofi-Aventis Deu...	Dermatop [®] base ointment	0F136A	1
Sanofi-Aventis Deu...	Dermatop [®] base ointment	9F183A	1
Sanofi/Gehe	Dermatop [®] base ointment	5F078A	1
Sanofi/GEHE	Dermatop [®] base ointment	8F117A	2
Sanofi/GEHE	Dermatop [®] base ointment	8F115A	1
Sanofi/Kehr	Dermatop [®] base ointment	6F099A	2
Sanofi/Noweda	Dermatop [®] base ointment	8F123B	3
Sanofi/Noweda	Dermatop [®] base ointment	8F126A	7
Sanofi/Noweda	Dermatop [®] base ointment	9F132A	1
Sanofi/Noweda	Dermatop [®] base ointment	0F138A	23
Sanofi/Noweda	Dermatop [®] base ointment	0F143A	31
Sanofi/Noweda	Dermatop [®] base ointment	0F142A	3
Sanofi/Noweda	Dermatop [®] base ointment	1F147A	1
Sanofi/Noweda	Dermatop [®] base ointment	1F146A	5
Sanofi/Noweda	Dermatop [®] base ointment	F144A	1
Sanofi/Noweda	Dermatop [®] base ointment	1F154A	1
Sanofi/Phoenix	Dermatop [®] base ointment	8F120A	2
Sanofi/Phoenix	Dermatop [®] base ointment	1F151A	2
Sanofi/Phönix	Dermatop [®] base ointment	7F105A	1
Sanofi/Phönix	Dermatop [®] base ointment	7F109A	2

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Supplier	Substance	Batch	Spectra
Sanofi/Phönix	Dermatop [®] base ointment	8F113A	1
Sanofi/Phönix	Dermatop [®] base ointment	8F114A	1
Sanofi/Phönix	Dermatop [®] base ointment	8F116A	3
Sanofi/Phönix	Dermatop [®] base ointment	8F118B	2
Sanofi/Phönix	Dermatop [®] base ointment	8F119A	4
Sanofi/Phönix	Dermatop [®] base ointment	8F121A	5
Sanofi/Phönix	Dermatop [®] base ointment	8F1238	1
Sanofi/Phönix	Dermatop [®] base ointment	F137A	2
Sanofi/Phönix	Dermatop [®] base ointment	F139A	4
sanofi/Sanacorp	Dermatop [®] base ointment	F135A	1
Sanofi/Sanacorp	Dermatop [®] base ointment	9F133A	4
Allergika Pharma GmbH	Dermifant [®] kids cream 20% MED	1410072	1
Allergika Pharma, Gehe	Dermifant [®] kids cream 20% MED	1604021	1
Allergika Pharma/A...	Dermifant [®] kids cream 20% MED	1511052	1
Allergika/ GEHE	Dermifant [®] kids cream 20% MED	1609042	3
Allergika/ GEHE	Dermifant [®] kids cream 20% MED	1612055	2
Allergika/ GEHE	Dermifant [®] kids cream 20% MED	1702011	1
Allergika/Gehe	Dermifant [®] kids cream 20% MED	1502013	1
Allergika/Phönix	Dermifant [®] kids cream 20% MED	1509042	1
Fagron	Dermifant [®] kids cream 20% MED	1705043	3
Gehe	Dermifant [®] kids cream 20% MED	1407053	1
Gehe	Dermifant [®] kids cream 20% MED	1803060	1
Gehe	Dermifant [®] kids cream 20% MED	1807083	1
Gehe	Dermifant [®] kids cream 20% MED	1810091	1
Phönix	Dermifant [®] kids cream 20% MED	1312102	2
Phönix EK:10,19 ...	Dermifant [®] kids cream 20% MED	1703024	1
Sanacorp WE: 09.11...	Dermifant [®] kids cream 20% MED	1708063	2
Sanacorp7Mida WE:...	Dermifant [®] kids cream 20% MED	1711094	4
Allergika/Kehr	Dermifant [®] kids lotion	1604060	1
Sanacorp EK:10,80...	Dermifant [®] kids lotion	1705111	1
Deumavan/Phoenix	Deumavan [®] protection ointme...	21710920	2
Kaymogyn GmbH / Phoenix	Deumavan [®] protection ointme...	L0T25620721	1
	Dexeryl [®]	3G5AF	1
Alliance	Dexeryl [®]	3SGTD	2
Noweda	Dexeryl [®]	G00909	1
P.Fabre/Phoenix	Dexeryl [®]	G00951	1
Phoenix	Dexeryl [®]	3SGTF	1
PiereFabre/Now	Dexeryl [®]	G00577	1
Pierre Fabre / phoenix	Dexeryl [®]	600869	1
Pierre Fabre /Noweda	Dexeryl [®]	G00606	1
Pierre Fabre/Now	Dexeryl [®]	G00650	1
Pierre Fabre/Sanacorp	Dexeryl [®]	G00729	2
Pierre Fabre/Sanacorp	Dexeryl [®]	G00064_A	1
PierreFabre/ Phoenix	Dexeryl [®]	G00835	1
PierreFabre/ Phoenix	Dexeryl [®]	G00904	1
PierreFabre/ Phoenix	Dexeryl [®]	G00966	2
PierreFabre/ Phoenix	Dexeryl [®]	G00967	2
PierreFabre/ Phoenix	Dexeryl [®]	G00956/2x500g	1
PierreFabre/ Phoenix	Dexeryl [®]	G01021	2
PierreFabre/ Phoenix	Dexeryl [®]	G01088	1
PierreFabre/ Phoenix	Dexeryl [®]	G01118	1
PierreFabre/ Phoenix	Dexeryl [®]	G01117	1
PierreFabre/ Phoenix	Dexeryl [®]	G01122	1
koko	DMS [®] base cream classic	L020E18	1
Koko	DMS [®] base cream classic	L042K24	1

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Supplier	Substance	Batch	Spectra
KOKO	DMS [®] base cream classic	L022S19	3
KOKO	DMS [®] base cream classic	L026A20	1
KOKO	DMS [®] base cream classic	L079E21	1
KOKO direkt	DMS [®] base cream classic	L036L20	2
KOkO GmbH	DMS [®] base cream classic	801010	1
KOKO GmbH	DMS [®] base cream classic	L005A14	1
KOKO GmbH	DMS [®] base cream classic	L003E16	1
KOKO GmbH & Co KG	DMS [®] base cream classic	L062H18	6
KOKO GmbH & Co KG	DMS [®] base cream classic	L036I18	2
KOKO GmbH & Co KG	DMS [®] base cream classic	L036118	2
KOKO GmbH & Co KG	DMS [®] base cream classic	L036118	1
koko GmbH EK: EUR	DMS [®] base cream classic	L008F17	1
38...			
KoKo GmbH/KoKo GmbH	DMS [®] base cream classic	11090E19	1
KoKo GmbH/KoKo GmbH	DMS [®] base cream classic		1
Koko GmbH&Co KG	DMS [®] base cream classic	L038J16	1
KOKO GmbH&Co.KG	DMS [®] base cream classic	L075G19	1
Caelo	DMS [®] base cream high classic	L010J15	1
Caelo	DMS [®] base cream high classic	L047I17	4
koko	DMS [®] base cream high classic	L001F17	1
koko	DMS [®] base cream high classic	L006K17	1
Koko	DMS [®] base cream high classic	L034F21	1
Koko	DMS [®] base cream high classic	L042K24	1
KOKO	DMS [®] base cream high classic	L035D19	1
KOKO	DMS [®] base cream high classic	L013F19	1
KOKO	DMS [®] base cream high classic	L035L19	2
KOKO	DMS [®] base cream high classic	L048L19	3
KOKO	DMS [®] base cream high classic	L014C20	1
KOKO	DMS [®] base cream high classic	L045T20	1
KOKO	DMS [®] base cream high classic	L057S20	1
KOKO	DMS [®] base cream high classic	L079K20	2
KOKO	DMS [®] base cream high classic	L047K20	1
KOKO	DMS [®] base cream high classic	L033C21	1
KOKO	DMS [®] base cream high classic	L045G21	3
KOKO	DMS [®] base cream high classic	L066A22	1
KOKO	DMS [®] base cream high classic	L065D22	1
KOKO	DMS [®] base cream high classic	L065d22	1
KOKO	DMS [®] base cream high classic	L081F22	1
Koko GmbH	DMS [®] base cream high classic	L019H17	6
Koko GmbH	DMS [®] base cream high classic	L033J17	3
Koko GmbH	DMS [®] base cream high classic	L031D18	1
Koko GmbH	DMS [®] base cream high classic	L031A14	2
Koko GmbH	DMS [®] base cream high classic	L050J18	2
Koko GmbH	DMS [®] base cream high classic	L064C24	2
KOKO GmbH	DMS [®] base cream high classic	L010E17	10
KOKO GmbH	DMS [®] base cream high classic	L008K17	5
KOKO GmbH	DMS [®] base cream high classic	1028c18	5
KOKO GmbH	DMS [®] base cream high classic	L042E18	5
KOKO GmbH	DMS [®] base cream high classic	1053f18	3
KOKO GmbH	DMS [®] base cream high classic	L050I18	5
KOKO GmbH	DMS [®] base cream high classic	L004K18	4
KOKO GmbH	DMS [®] base cream high classic	L002B19	5
KOKO GmbH	DMS [®] base cream high classic	L012G19	3
KOKO GmbH	DMS [®] base cream high classic	1o74s19	2
KOKO GmbH	DMS [®] base cream high classic	L035L19	2

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Supplier	Substance	Batch	Spectra
KOKO GmbH	DMS [®] base cream high classic	L014C20	4
KOKO GmbH	DMS [®] base cream high classic	L015H20	5
KOKO GmbH	DMS [®] base cream high classic	L034F21	4
KOKO GmbH	DMS [®] base cream high classic	L030L16	3
KOKO GmbH & Co. KG	DMS [®] base cream high classic	L054B16	1
Koko Kosmetik	DMS [®] base cream high classic	L080B25	1
koko	DMS [®] base cream high classi...	L047T24	1
Koko	DMS [®] base cream high classi...	L009F21	2
Koko	DMS [®] base cream high classi...	L083S21	3
KoKo	DMS [®] base cream high classi...	L014C16	1
KOKO	DMS [®] base cream high classi...	80304101	1
KOKO	DMS [®] base cream high classi...	L026A19	1
KOKO	DMS [®] base cream high classi...	L071T20	1
KOKO	DMS [®] base cream high classi...	L063A21	2
KOKO	DMS [®] base cream high classi...	L037B21	2
KOKO	DMS [®] base cream high classi...	L089G21	3
KOKO	DMS [®] base cream high classi...	L017E22	1
Koko GmbH	DMS [®] base cream high classi...	L035F17	1
Koko GmbH	DMS [®] base cream high classi...	L072E19	1
Koko GmbH	DMS [®] base cream high classi...	L028A20	2
Koko GmbH	DMS [®] base cream high classi...	L063H20	2
Koko GmbH	DMS [®] base cream high classi...	L017S24	1
KOKO GmbH & Co. KG	DMS [®] base cream high classi...	L018D16	1
KoKo GmbH&Co.KG	DMS [®] base cream high classi...	L013K16	3
KoKo GmbH&Co.KG	DMS [®] base cream high classi...	L016D17	3
KoKo GmbH&Co.KG	DMS [®] base cream high classi...	L035K17	1
KoKo GmbH&Co.KG	DMS [®] base cream high classi...	L030A18	2
KoKo GmbH&Co.KG	DMS [®] base cream high classi...	L034C18	1
KoKo GmbH&Co.KG	DMS [®] base cream high classi...	L030G18	2
KoKo GmbH&Co.KG	DMS [®] base cream high classi...	L030G18	1
KoKo GmbH&Co.KG	DMS [®] base cream high classi...	L027T19	1
Koko Kosmetik	DMS [®] base cream high classi...	L041C25	2

E

Supplier	Substance	Batch	Spectra
Beiersdorf	Eucerinum O/W basis	24830308WA	2
Beiersdorf	Eucerinum O/W basis	319030108WA	1
Beiersdorf	Eucerinum O/W basis	41830108WA	1
Beiersdorf	Eucerinum O/W basis	51630108WA	1
Beiersdorf	Eucerinum O/W basis	51630108WA	3
Beiersdorf	Eucerinum O/W basis	61130108WA	2
Beiersdorf	Eucerinum O/W basis	72630108WA	2
Beiersdorf	Eucerinum O/W basis	8373038WA	1
Beiersdorf	Eucerinum O/W basis	94830308WA	4
Beiersdorf /Noweda	Eucerinum O/W basis	94830108wa	1
Beiersdorf AG	Eucerinum O/W basis	2483030308WA	1
Beiersdorf AG/Noweda	Eucerinum O/W basis	53430208WA	2
Beiersdorf,Gehe	Eucerinum O/W basis	94830108WA	10
Beiersdorf/ Phoenix	Eucerinum O/W basis	80230108WA	4
Beiersdorf/ Phoenix	Eucerinum O/W basis	84030208Wa	1
Beiersdorf/Kehr	Eucerinum O/W basis	53430208WA	5
Beiersdorf/Noweda	Eucerinum O/W basis	84030108WA	7
Beiersdorf/Sanacorp	Eucerinum O/W basis	84030208WA	11
Caelo	Eucerinum O/W basis	31930108WA	3
Caelo	Eucerinum O/W basis	64030208WA	5
Caelo	Eucerinum O/W basis	13730308WA	1

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Supplier	Substance	Batch	Spectra
Allianz Healthcare	Eucerinum W/O basis	64030108wa	1
Caelo	Eucerinum W/O basis	53430208WA	16
Baiersdorf	Eucerinum W/O basis	41839108WA	1
Baiersdorf	Eucerinum W/O basis	43430208WA	3
Beiersdor	Eucerinum W/O basis	541830108WA	1
Beiersdorf	Eucerinum W/O basis	21430108WA	4
Beiersdorf	Eucerinum W/O basis	24830208WA	3
Beiersdorf	Eucerinum W/O basis	32930208WA	9
Beiersdorf	Eucerinum W/O basis	31230108wa	1
Beiersdorf	Eucerinum W/O basis	34930308WA	10
Beiersdorf	Eucerinum W/O basis	24072015A	1
Beiersdorf	Eucerinum W/O basis	516301328wa	1
Beiersdorf	Eucerinum W/O basis	438679	1
Beiersdorf	Eucerinum W/O basis	80339108WA	1
Beiersdorf	Eucerinum W/O basis	83730208WA	29
Beiersdorf	Eucerinum W/O basis	94930208	38
Beiersdorf	Eucerinum W/O basis	94980208	1
Beiersdorf / Allia...	Eucerinum W/O basis	949301018	1
Beiersdorf / Phoenix	Eucerinum W/O basis	80330108WA	25
Beiersdorf AG	Eucerinum W/O basis	53630108WA	1
Beiersdorf AG	Eucerinum W/O basis	3730208WA	1
Beiersdorf AG	Eucerinum W/O basis	94930108	34
Beiersdorf/ Alliance	Eucerinum W/O basis	949330208	1
Beiersdorf/ Sanacorp	Eucerinum W/O basis	418301087WA	1
Beiersdorf/ Sanacorp	Eucerinum W/O basis	94930308	9
Beiersdorf/Anzag	Eucerinum W/O basis	1(83730208WA)	1
Beiersdorf/Anzag	Eucerinum W/O basis	211202(94930308)	1
Beiersdorf/Geibo	Eucerinum W/O basis	94930208WA	1
Beiersdorf/Kehr	Eucerinum W/O basis	80330108	1
Beiersdorf/Noweda	Eucerinum W/O basis	41830108Wa	1
Beiersdorf/Noweda	Eucerinum W/O basis	51630108wa	2
Beiersdorf/Noweda	Eucerinum W/O basis	53430288WA	1
Beiersdorf/Noweda	Eucerinum W/O basis	64030108WA	11
Beiersdorf/Noweda	Eucerinum W/O basis	72630108VVA	1
Beiersdorf/Noweda	Eucerinum W/O basis	726300108WA	1
Beiersdorf/Noweda	Eucerinum W/O basis	83730308WA	13
Beiersdorf/Phoenix	Eucerinum W/O basis	83730206WA	2
Beiersdorf/Phoenix	Eucerinum W/O basis	94930108WA	1
Beiersdorf/Phoenix	Eucerinum W/O basis	94920208	1
Beiersdorf/Sanacorp	Eucerinum W/O basis	31230108WA	8
Caelo	Eucerinum W/O basis	72630108Wa	1
Caelo	Eucerinum W/O basis	51630108	1
eucerinum	Eucerinum W/O basis	41830108WA	11
Gehe/Beiersdorf	Eucerinum W/O basis	51630108WA	28
Noweda	Eucerinum W/O basis	72630108WA	20
Noweda	Eucerinum W/O basis	8373C208WA	1
	Excipial [®] almond oil ointment	3774007	4
	Excipial [®] almond oil ointment	3774006	1
	Excipial [®] almond oil ointment	3774014	1
Caelo	Excipial [®] almond oil ointment	16106712	1
Caelo	Excipial [®] almond oil ointment	1otno32	1
Caelo	Excipial [®] almond oil ointment	20170829Ma2	1
Caelo	Excipial [®] almond oil ointment	20170829Ma3	1
Fiebig	Excipial [®] almond oil ointment	S051	1
galderma	Excipial [®] almond oil ointment	L0TT061	3
Galderma	Excipial [®] almond oil ointment	T051	2
Galderma	Excipial [®] almond oil ointment	T061	2
Galderma	Excipial [®] almond oil ointment	V011	6
Galderma	Excipial [®] almond oil ointment	L0TV011	2

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Supplier	Substance	Batch	Spectra
Galderma	Excipial [®] almond oil ointment	T011	1
Galderma	Excipial [®] almond oil ointment	V041	2
Galderma	Excipial [®] almond oil ointment	V042	3
Galderma	Excipial [®] almond oil ointment	V051	11
Galderma	Excipial [®] almond oil ointment	50498	10
Galderma	Excipial [®] almond oil ointment	50696	20
Galderma	Excipial [®] almond oil ointment	50238	2
Galderma	Excipial [®] almond oil ointment	8774007	3
Galderma	Excipial [®] almond oil ointment	8774006	6
Galderma	Excipial [®] almond oil ointment	9774001	17
Galderma	Excipial [®] almond oil ointment	9774002	4
Galderma	Excipial [®] almond oil ointment	9774006	10
Galderma	Excipial [®] almond oil ointment	9774007	11
Galderma	Excipial [®] almond oil ointment	774002	13
Galderma	Excipial [®] almond oil ointment	774005	1
Galderma	Excipial [®] almond oil ointment	774004	17
Galderma	Excipial [®] almond oil ointment	774009	10
Galderma	Excipial [®] almond oil ointment	10774009	1
Galderma	Excipial [®] almond oil ointment	774006	2
Galderma	Excipial [®] almond oil ointment	774010	12
Galderma	Excipial [®] almond oil ointment	1774002	7
Galderma	Excipial [®] almond oil ointment	1774007	9
Galderma	Excipial [®] almond oil ointment	774014	1
Galderma Internati...	Excipial [®] almond oil ointment	T031	2
Galderma Laborator...	Excipial [®] almond oil ointment	2774006	3
Galderma Laborator...	Excipial [®] almond oil ointment	1774009	11
Galderma-Spirig	Excipial [®] almond oil ointment	V042-20171127Ma12	1
Galderma/Anzag	Excipial [®] almond oil ointment	S033	1
Galderma/Anzag	Excipial [®] almond oil ointment	9774004	4
Galderma/Kehr	Excipial [®] almond oil ointment	V031	11
Galderma/Now	Excipial [®] almond oil ointment	L0TS021	1
Galderma/Noweda	Excipial [®] almond oil ointment	S012	1
Galderma/Phoenix	Excipial [®] almond oil ointment	T021	1
Galderma/Phoenix	Excipial [®] almond oil ointment	T041	1
Galderma/Phoenix	Excipial [®] almond oil ointment	8774005	8
Galderma/Phönix	Excipial [®] almond oil ointment	S021	3
Galderma/Phönix	Excipial [®] almond oil ointment	50239	7
Gehe	Excipial [®] almond oil ointment	1774008	1
Junek GmbH	Excipial [®] almond oil ointment	774001	1
Noweda	Excipial [®] almond oil ointment	8774004	4
Noweda	Excipial [®] almond oil ointment	9774003	6
Noweda	Excipial [®] almond oil ointment	9774005	7
Phoenix	Excipial [®] almond oil ointment	L0TN022	2
Spirig	Excipial [®] almond oil ointment	M032	1
Spirig	Excipial [®] almond oil ointment	L0TM023	1
Spirig	Excipial [®] almond oil ointment	N031	2
Spirig	Excipial [®] almond oil ointment	N032	1
Spirig	Excipial [®] almond oil ointment	M023	1
Spirig	Excipial [®] almond oil ointment	R012	2
Spirig	Excipial [®] almond oil ointment	S032	1
Spirig	Excipial [®] almond oil ointment	S011	1
Spirig / Galderma ...	Excipial [®] almond oil ointment	V061	3
Spirig / Gehe	Excipial [®] almond oil ointment	L0TN022	1
Spirig /Noweda	Excipial [®] almond oil ointment	r021	1
Spirig Pharma/Nowed	Excipial [®] almond oil ointment	N022	1
Spirig/AHD	Excipial [®] almond oil ointment	N011	1

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Supplier	Substance	Batch	Spectra
Spirig/Noweda	Excipial [®] almond oil ointment	R043	4
Spirig/Sanacorp	Excipial [®] almond oil ointment	L0TN011	1
	Excipial [®] hydro cream	C372	17
	Excipial [®] hydro cream	P201430-0	3
	Excipial [®] hydro cream	D492	6
	Excipial [®] hydro cream	E233	7
	Excipial [®] hydro cream	F.I.L0767	1
	Excipial [®] hydro cream	G372	1
	Excipial [®] hydro cream	B362	1
	Excipial [®] hydro cream	H154	3
	Excipial [®] hydro cream	I3041	4
Alliance/Spirig	Excipial [®] hydro cream	N043	1
Audor Pharma	Excipial [®] hydro cream	S056	1
Caelo	Excipial [®] hydro cream	V031	2
Caelo	Excipial [®] hydro cream	R045	1
Chiesi/Phoenix	Excipial [®] hydro cream	L0TV071	2
Fa.Gehe	Excipial [®] hydro cream	20160727Ma3	1
Galderma	Excipial [®] hydro cream	S054	5
Galderma	Excipial [®] hydro cream	L0TV071	2
Galderma	Excipial [®] hydro cream	L0TV051	1
Galderma	Excipial [®] hydro cream	L0TV072	1
Galderma	Excipial [®] hydro cream	50782	15
Galderma	Excipial [®] hydro cream	50634	3
Galderma	Excipial [®] hydro cream	50564	3
Galderma	Excipial [®] hydro cream	1767001	5
Galderma	Excipial [®] hydro cream	D432	1
Galderma /	Excipial [®] hydro cream	P28013-0	1
Galderma /Noweda	Excipial [®] hydro cream	1767002	7
Galderma /Phönix	Excipial [®] hydro cream	L0TT052	2
Galderma International	Excipial [®] hydro cream	A272	6
Galderma International	Excipial [®] hydro cream	c372	1
Galderma Laborator...	Excipial [®] hydro cream	9767006	3
Galderma-Spirig	Excipial [®] hydro cream	To52-20171127Ma11	1
Galderma-Spirig	Excipial [®] hydro cream	V041-20180619Ma8	1
Galderma-Spirig	Excipial [®] hydro cream	50235-E20190115Ma10	1
Galderma-Spirig,Ge...	Excipial [®] hydro cream	V061-20180830Ma11	1
Galderma/	Excipial [®] hydro cream	S012	1
Galderma/	Excipial [®] hydro cream	V011	1
Galderma/ Gehe	Excipial [®] hydro cream	V051	4
Galderma/ Noweda	Excipial [®] hydro cream	L0T50782	3
Galderma/Alliance	Excipial [®] hydro cream	T052	7
Galderma/Alliance ...	Excipial [®] hydro cream	S025	1
Galderma/Ebert	Excipial [®] hydro cream	V041	1
Galderma/Galderma	Excipial [®] hydro cream	S024	3
Galderma/Galderma	Excipial [®] hydro cream	so25	1
Galderma/Gehe	Excipial [®] hydro cream	R031	2
Galderma/Gehe	Excipial [®] hydro cream	V071	5
Galderma/Gehe	Excipial [®] hydro cream	V072	3
Galderma/Gehe	Excipial [®] hydro cream	8767001	2
Galderma/Gehe	Excipial [®] hydro cream	9757001	1
Galderma/Noweda	Excipial [®] hydro cream	170420EH/L0TT012	1
Galderma/Noweda	Excipial [®] hydro cream	170706EH/L0TT091	1
Galderma/Noweda	Excipial [®] hydro cream	V042	3
Galderma/Noweda	Excipial [®] hydro cream	180319EH/L0TV051	1
Galderma/Noweda	Excipial [®] hydro cream	1767003	7
Galderma/phoenix	Excipial [®] hydro cream	L0TT012	1

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Supplier	Substance	Batch	Spectra
Galderma/Phoenix	Excipial [®] hydro cream	50235	3
Galderma/Phoenix	Excipial [®] hydro cream	50515	3
Galderma/Phoenix	Excipial [®] hydro cream	9767001	9
Galderma/Phoenix	Excipial [®] hydro cream	9767005	10
Galderma/Phoenix	Excipial [®] hydro cream	9767002	3
Galderma/Phoenix(1...	Excipial [®] hydro cream	1767003A	5
Galderma/Phönix	Excipial [®] hydro cream	V061	1
Galderma/Phönix	Excipial [®] hydro cream	S045	1
Galderma/Phönix	Excipial [®] hydro cream	S013	1
Galderma/Phönix	Excipial [®] hydro cream	T081	1
Galderma/Phönix	Excipial [®] hydro cream	V052	1
Galderma/Sanacorp	Excipial [®] hydro cream	LOTV041	1
Galderma/Sanacorp	Excipial [®] hydro cream	769013	1
Galderma/Sanacorp	Excipial [®] hydro cream	767001	7
Gehe, Galderma Spirig	Excipial [®] hydro cream	R031-20160615Ma7	1
Gladerma/Ebert	Excipial [®] hydro cream	V072	1
Noweda	Excipial [®] hydro cream	1120114	1
Noweda	Excipial [®] hydro cream	V051	1
Noweda	Excipial [®] hydro cream	767004	6
Noweda/Galderma	Excipial [®] hydro cream	T091	2
Phoenix/Spirig	Excipial [®] hydro cream	M015	1
Phoenix/Spirig	Excipial [®] hydro cream	N044	1
Phönix	Excipial [®] hydro cream	767003	2
Sanacorp	Excipial [®] hydro cream	LOTN011	1
Spirig Pharma AG/...	Excipial [®] hydro cream	LOTN034	1
Spirig Pharma AG/...	Excipial [®] hydro cream	LOTR013	1
spirig	Excipial [®] hydro cream	M014	2
spirig	Excipial [®] hydro cream	M034	1
spirig	Excipial [®] hydro cream	M041	1
spirig	Excipial [®] hydro cream	N014	1
spirig	Excipial [®] hydro cream	N043	6
spirig	Excipial [®] hydro cream	R013	4
spirig	Excipial [®] hydro cream	N045	2
spirig	Excipial [®] hydro cream	R014	4
spirig	Excipial [®] hydro cream	s025	1
Spirig	Excipial [®] hydro cream	K013	1
Spirig	Excipial [®] hydro cream	N035	1
Spirig	Excipial [®] hydro cream	S025	7
Spirig (Galderma)	Excipial [®] hydro cream	T012	3
Spirig / Anzag	Excipial [®] hydro cream	813993/09	1
Spirig / Anzag	Excipial [®] hydro cream	N034	4
Spirig / Anzag	Excipial [®] hydro cream	LOTN043	1
Spirig /Gehe	Excipial [®] hydro cream	LOTN044	1
Spirig Pharma	Excipial [®] hydro cream	N013	1
Spirig Pharma	Excipial [®] hydro cream	813993/10	3
Spirig Pharma	Excipial [®] hydro cream	N011	3
Spirig Pharma	Excipial [®] hydro cream	LON014	1
Spirig Pharma	Excipial [®] hydro cream	N044	1
Spirig Pharma AG	Excipial [®] hydro cream	813993/12	1
Spirig Pharma AG	Excipial [®] hydro cream	R025	5
Spirig Pharma AG/GEHE	Excipial [®] hydro cream	R011	4
Spirig Pharma/ G	Excipial [®] hydro cream	S053	1
Spirig Pharma/ Noweda	Excipial [®] hydro cream	N042	2
Spirig Pharma/Gehe	Excipial [®] hydro cream	3.02.2014	1
Spirig/Anzag	Excipial [®] hydro cream	LOTM041	1

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Supplier	Substance	Batch	Spectra
Spirig/Anzag	Excipial [®] hydro cream	N035	2
Spirig/Fiebig	Excipial [®] hydro cream	N013	1
Spirig/Gehe	Excipial [®] hydro cream	M012	1
Spirig/Gehe	Excipial [®] hydro cream	L0TR031	2
Spirig/Gehe	Excipial [®] hydro cream	R031, 20161215Ma4	1
Spirig/Gehe	Excipial [®] hydro cream	T052, 20170216Ma7	1
Spirig/Gehe	Excipial [®] hydro cream	T052, 20170216Ma8	1
Spirug Pharma AG/ GEHE	Excipial [®] hydro cream	V011	9
Spring Pharma AG/ GEHE	Excipial [®] hydro cream	T011	2
Spirig / Noweda	Excipial [®] hydro cream	S041	8
	Excipial [®] lipo cream	D372	5
	Excipial [®] lipo cream	L275	1
	Excipial [®] lipo cream	L283	2
	Excipial [®] lipo cream	L273	3
	Excipial [®] lipo cream	M473	3
	Excipial [®] lipo cream	Q074	12
	Excipial [®] lipo cream	R144	1
	Excipial [®] lipo cream	R154	4
	Excipial [®] lipo cream	Q027	1
	Excipial [®] lipo cream	V324	1
Alliance Healthcare	Excipial [®] lipo cream	M045	1
Alliance Healthcare	Excipial [®] lipo cream		5
Anzag/ Chiesi	Excipial [®] lipo cream	L0TR012	2
Caelo	Excipial [®] lipo cream	V112	4
Caelo	Excipial [®] lipo cream	9031	1
Caelo	Excipial [®] lipo cream	7121	1
galderma	Excipial [®] lipo cream	L0T50627	1
Galderma	Excipial [®] lipo cream	R012	2
Galderma	Excipial [®] lipo cream	R042	15
Galderma	Excipial [®] lipo cream	R035	2
Galderma	Excipial [®] lipo cream	L0TS032	1
Galderma	Excipial [®] lipo cream	T061	4
Galderma	Excipial [®] lipo cream	V051	3
Galderma	Excipial [®] lipo cream	v042	1
Galderma	Excipial [®] lipo cream	L0TV041	1
Galderma	Excipial [®] lipo cream	50567	15
Galderma	Excipial [®] lipo cream	9769010	4
Galderma	Excipial [®] lipo cream	9769005	2
Galderma	Excipial [®] lipo cream	1769001	10
Galderma	Excipial [®] lipo cream	2769006	15
Galderma /AHD	Excipial [®] lipo cream	8769004	8
Galderma Internati...	Excipial [®] lipo cream	769005	2
Galderma Laborator...	Excipial [®] lipo cream	1769020	7
Dermapharm	Excipial [®] lipo cream	1769022	6
Galderma/ Fiebig	Excipial [®] lipo cream	L0TV111	1
Galderma/ Noweda	Excipial [®] lipo cream	s023	6
Galderma/ Noweda	Excipial [®] lipo cream	t022	5
Galderma/ Noweda	Excipial [®] lipo cream	T022	4
Galderma/ Sanacorp	Excipial [®] lipo cream	L0T50567	1
Galderma/Alliance	Excipial [®] lipo cream	V091	4
Galderma/Alliance	Excipial [®] lipo cream	769013	9
Galderma/Anzag	Excipial [®] lipo cream	S011	1
Galderma/Galderma	Excipial [®] lipo cream	R026	1
Galderma/Galderma	Excipial [®] lipo cream	ro26	1

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Supplier	Substance	Batch	Spectra
Galderma/Galderma	Excipial [®] lipo cream	S023	10
Galderma/Galderma	Excipial [®] lipo cream	T021	18
Galderma/Galderma	Excipial [®] lipo cream	V121	1
Galderma/Gehe	Excipial [®] lipo cream	50849	5
Galderma/Gehe	Excipial [®] lipo cream	9769004	13
Galderma/Gehe	Excipial [®] lipo cream	769002	9
Galderma/Noweda	Excipial [®] lipo cream	R011	2
Galderma/Noweda	Excipial [®] lipo cream	170420EL/LOTT021	1
Galderma/Noweda	Excipial [®] lipo cream	171819E/LOTT021	1
Galderma/Noweda	Excipial [®] lipo cream	180208L/LOTV091	1
Galderma/Noweda	Excipial [®] lipo cream	9769030	15
Galderma/Noweda	Excipial [®] lipo cream	1769003	9
Galderma/Phönix	Excipial [®] lipo cream	R042	1
Galderma/Phönix	Excipial [®] lipo cream	S032	1
Galderma/Phönix	Excipial [®] lipo cream	9769011	6
Galderma/Phönix	Excipial [®] lipo cream	LOTV012	1
WE. . .			
Galderma/Sanacorp	Excipial [®] lipo cream	1769017	12
Galderma/Sanacorp	Excipial [®] lipo cream	1769014	4
Galderma/Sanacorp	Excipial [®] lipo cream	E412	13
Galmeda Noweda	Excipial [®] lipo cream	180504EL/LOTV112	1
Gehe	Excipial [®] lipo cream	N061	5
Gehe	Excipial [®] lipo cream	Q074	1
Gehe/Galderma	Excipial [®] lipo cream	L0TS031	1
Nestle Skin Health	Excipial [®] lipo cream	311839	1
Noweda	Excipial [®] lipo cream	50627	5
Noweda/ Galderma	Excipial [®] lipo cream	V112180607EL	1
Caelo	Excipial [®] lipo cream	L0TS023	1
Phönix/Galderma	Excipial [®] lipo cream	S023	1
Sanacorp	Excipial [®] lipo cream	M027	1
Sanacorp	Excipial [®] lipo cream	LOTN016	1
spirig	Excipial [®] lipo cream	M017	3
spirig	Excipial [®] lipo cream	M016	4
spirig	Excipial [®] lipo cream	M041	7
spirig	Excipial [®] lipo cream	N021	6
spirig	Excipial [®] lipo cream	r042	1
Spirig	Excipial [®] lipo cream	K021	1
Spirig	Excipial [®] lipo cream	R012	12
Spirig / Anzag	Excipial [®] lipo cream	N018	10
Spirig / Anzag	Excipial [®] lipo cream	N018	1
Spirig /Gehe	Excipial [®] lipo cream	LOTN021	4
Spirig /Gehe	Excipial [®] lipo cream	L0TR012	1
Spirig Pharma	Excipial [®] lipo cream	813994/09	4
Spirig Pharma Euro...	Excipial [®] lipo cream	R026	8
Spirig/Phoenix	Excipial [®] lipo cream	M042	8
Spirig/Phönix	Excipial [®] lipo cream	4622	1
Spirig Pharma AG ...	Excipial [®] lipo cream	L0TS011	1
Wolff	Excipial [®] lipo cream	S031	12
	Excipial [®] U Hydrolotio	378787	8
	Excipial [®] U Hydrolotio	394125	3
	Excipial [®] U Hydrolotio	401464	2
Alliance	Excipial [®] U Hydrolotio	T012	1
Caelo	Excipial [®] U Hydrolotio	L0TR092	1
Galderma	Excipial [®] U Hydrolotio	L0TR054	1
Galderma	Excipial [®] U Hydrolotio	T011	1
Galderma	Excipial [®] U Hydrolotio	50857	1

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Supplier	Substance	Batch	Spectra
Galderma	Excipial [®] U Hydrolotio	1107483	1
Galderma	Excipial [®] U Hydrolotio	302972	3
Galderma	Excipial [®] U Hydrolotio	315815	2
Galderma	Excipial [®] U Hydrolotio	318203	1
Galderma Internati...	Excipial [®] U Hydrolotio	346815	2
Galderma Internati...	Excipial [®] U Hydrolotio	V042	2
Galderma Laborator...	Excipial [®] U Hydrolotio	318208	1
Galderma Laborator...	Excipial [®] U Hydrolotio	344143	6
Galderma/ Fiebig	Excipial [®] U Hydrolotio	L0TV022	1
Galderma/ Gehe	Excipial [®] U Hydrolotio	L0TR053	1
Galderma/ Phoenix	Excipial [®] U Hydrolotio	344145	2
Galderma/ Phoenix/...	Excipial [®] U Hydrolotio	327533	2
Galderma/AEP	Excipial [®] U Hydrolotio	324226	2
Galderma/Alliance	Excipial [®] U Hydrolotio	T072	2
Galderma/Alliance	Excipial [®] U Hydrolotio	50723	2
Galderma/Alliance	Excipial [®] U Hydrolotio	365111	5
Galderma/Anzag	Excipial [®] U Hydrolotio	1(172141)	1
Galderma/Anzag	Excipial [®] U Hydrolotio	2(302972)	1
Galderma/Anzag	Excipial [®] U Hydrolotio	3(302972)	1
Galderma/Anzag	Excipial [®] U Hydrolotio	4(302972)	1
Galderma/Anzag	Excipial [®] U Hydrolotio	5(302972)	1
Galderma/Anzag	Excipial [®] U Hydrolotio	6(317160)	1
Galderma/Gehe	Excipial [®] U Hydrolotio	S014	1
Galderma/Gehe	Excipial [®] U Hydrolotio	V052	1
Galderma/Gehe	Excipial [®] U Hydrolotio	164957	3
Galderma/Noweda	Excipial [®] U Hydrolotio	340006	1
Galderma/Noweda	Excipial [®] U Hydrolotio	357789	2
galderma/phönix	Excipial [®] U Hydrolotio	332020	1
Galderma/Phönix	Excipial [®] U Hydrolotio	T013	1
Galderma/Phönix	Excipial [®] U Hydrolotio	V011	1
Galderma/Sanacorp	Excipial [®] U Hydrolotio	340781	5
Nestle Skin Health...	Excipial [®] U Hydrolotio	324614	5
Nestle Skin Health...	Excipial [®] U Hydrolotio	331554	10
Nestle Skinhealth/Gehe	Excipial [®] U Hydrolotio	172481	3
Nestle Skinhealth/Gehe	Excipial [®] U Hydrolotio	173466	1
Nestle Skinhealth/Gehe	Excipial [®] U Hydrolotio	306123	3
Nestle Skinhealth/Sana	Excipial [®] U Hydrolotio	312920	2
Noweda	Excipial [®] U Hydrolotio	S061	1
Phoenix/Spirig	Excipial [®] U Hydrolotio	M016	1
PHÖNIX	Excipial [®] U Hydrolotio	V051	2
PHÖNIX	Excipial [®] U Hydrolotio	50593	1
Phönix, Galderma, ...	Excipial [®] U Hydrolotio	317160	1
SANACORP	Excipial [®] U Hydrolotio	172141	1
Spirig	Excipial [®] U Hydrolotio	N013	1
Spirig	Excipial [®] U Hydrolotio	N013	1
Spirig Pharma	Excipial [®] U Hydrolotio	N033	1
Spirig Pharma AG/ ...	Excipial [®] U Hydrolotio	L0TN022	1
Spirig/Gehe	Excipial [®] U Hydrolotio	R054	5
	Excipial [®] U Lipolotio	378835	3
	Excipial [®] U Lipolotio	363077	2
	Excipial [®] U Lipolotio	378788	1
	Excipial [®] U Lipolotio	381338	3
	Excipial [®] U Lipolotio	375948	1
	Excipial [®] U Lipolotio	375353	1
	Excipial [®] U Lipolotio	381761	6
	Excipial [®] U Lipolotio	386055	4

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Supplier	Substance	Batch	Spectra
	Excipial [®] U Lipolotio	383121	7
	Excipial [®] U Lipolotio	385639	1
	Excipial [®] U Lipolotio	385490	3
	Excipial [®] U Lipolotio	393121	1
	Excipial [®] U Lipolotio	378789	2
	Excipial [®] U Lipolotio	384503	1
	Excipial [®] U Lipolotio	387279	2
	Excipial [®] U Lipolotio	371408	4
	Excipial [®] U Lipolotio	100121	1
	Excipial [®] U Lipolotio	371409	3
	Excipial [®] U Lipolotio	400121	5
	Excipial [®] U Lipolotio	396254	3
	Excipial [®] U Lipolotio	389197	2
	Excipial [®] U Lipolotio	388932	1
	Excipial [®] U Lipolotio	385487	3
	Excipial [®] U Lipolotio	394130	2
	Excipial [®] U Lipolotio	397664	4
	Excipial [®] U Lipolotio	406205	1
	Excipial [®] U Lipolotio	401447	4
	Excipial [®] U Lipolotio	389196	1
	Excipial [®] U Lipolotio	402396	1
	Excipial [®] U Lipolotio	402679	5
	Excipial [®] U Lipolotio	409451	2
Caelo	Excipial [®] U Lipolotio	R186	1
Caelo	Excipial [®] U Lipolotio	V143	2
Caelo	Excipial [®] U Lipolotio	18023004	2
Caelo	Excipial [®] U Lipolotio	LotV137	1
Caelo	Excipial [®] U Lipolotio	LoTV143	1
Caelo	Excipial [®] U Lipolotio	173048	2
Caelo	Excipial [®] U Lipolotio	S073	1
Caesar & Loretz GmbH	Excipial [®] U Lipolotio	19065102	1
Caleo/Alliance	Excipial [®] U Lipolotio	50791	2
Chiesi	Excipial [®] U Lipolotio	S116	1
Euro/ Phönix	Excipial [®] U Lipolotio	4417A-03749	1
Fagron	Excipial [®] U Lipolotio	N168	2
Fagron	Excipial [®] U Lipolotio	T123	1
Fagron	Excipial [®] U Lipolotio	V081	1
Fiebig/DR.Wolf	Excipial [®] U Lipolotio	V028	1
Fiebig/Galderma	Excipial [®] U Lipolotio	V101	3
Fischar	Excipial [®] U Lipolotio	LOTN085	1
Galaderma	Excipial [®] U Lipolotio	R072	1
Galaderma/Krieger	Excipial [®] U Lipolotio	V011	2
Galaderma/Krieger	Excipial [®] U Lipolotio	LOT50249	1
Galaderma/Krieger	Excipial [®] U Lipolotio	LOT50842	1
Galaderma/Phönix	Excipial [®] U Lipolotio	LOTV152	1
galderma	Excipial [®] U Lipolotio	R024	1
Galderma	Excipial [®] U Lipolotio	R111	1
Galderma	Excipial [®] U Lipolotio	R115	1
Galderma	Excipial [®] U Lipolotio	R167	4
Galderma	Excipial [®] U Lipolotio	R168	1
Galderma	Excipial [®] U Lipolotio	S064	1
Galderma	Excipial [®] U Lipolotio	S091	2
Galderma	Excipial [®] U Lipolotio	S065	1
Galderma	Excipial [®] U Lipolotio	R172	1
Galderma	Excipial [®] U Lipolotio	S137	1
Galderma	Excipial [®] U Lipolotio	S147	2

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Supplier	Substance	Batch	Spectra
Galderma	Excipial [®] U Lipolotio	R143	1
Galderma	Excipial [®] U Lipolotio	T056	1
Galderma	Excipial [®] U Lipolotio	T125	2
Galderma	Excipial [®] U Lipolotio	T062	1
Galderma	Excipial [®] U Lipolotio	V011	2
Galderma	Excipial [®] U Lipolotio	L0TS123	1
Galderma	Excipial [®] U Lipolotio	V037	1
Galderma	Excipial [®] U Lipolotio	L0TV121	1
Galderma	Excipial [®] U Lipolotio	T085	2
Galderma	Excipial [®] U Lipolotio	V139	2
Galderma	Excipial [®] U Lipolotio	V025	1
Galderma	Excipial [®] U Lipolotio	V153	2
Galderma	Excipial [®] U Lipolotio	V159	1
Galderma	Excipial [®] U Lipolotio	50458	1
Galderma	Excipial [®] U Lipolotio	V161	1
Galderma	Excipial [®] U Lipolotio	50295	1
Galderma	Excipial [®] U Lipolotio	50346	1
Galderma	Excipial [®] U Lipolotio	50852	9
Galderma	Excipial [®] U Lipolotio	270918A	1
Galderma	Excipial [®] U Lipolotio	169010	6
Galderma	Excipial [®] U Lipolotio	169853	5
Galderma	Excipial [®] U Lipolotio	169005	1
Galderma	Excipial [®] U Lipolotio	304310	1
Galderma	Excipial [®] U Lipolotio	308637	9
Galderma	Excipial [®] U Lipolotio	311839	13
Galderma	Excipial [®] U Lipolotio	319921	5
Galderma	Excipial [®] U Lipolotio	319351	3
Galderma	Excipial [®] U Lipolotio	323922	8
Galderma	Excipial [®] U Lipolotio	324788	5
Galderma	Excipial [®] U Lipolotio	327343	9
Galderma	Excipial [®] U Lipolotio	326881	9
Galderma	Excipial [®] U Lipolotio	334288	5
Galderma	Excipial [®] U Lipolotio	338630	3
Galderma	Excipial [®] U Lipolotio	339852	4
Galderma	Excipial [®] U Lipolotio	344109	7
Galderma	Excipial [®] U Lipolotio	355168	1
Galderma	Excipial [®] U Lipolotio	335167	1
Galderma	Excipial [®] U Lipolotio	357791	6
Galderma	Excipial [®] U Lipolotio	351025	1
Galderma	Excipial [®] U Lipolotio	356830	1
Galderma	Excipial [®] U Lipolotio	363070	1
Galderma (Spirig P...	Excipial [®] U Lipolotio	R061	1
Galderma (Spirig P...	Excipial [®] U Lipolotio	T057	1
Galderma / Galderma	Excipial [®] U Lipolotio	R086	1
Galderma / Kehr	Excipial [®] U Lipolotio	R171	3
Galderma / Kehr	Excipial [®] U Lipolotio	T029	2
Galderma / Kehr	Excipial [®] U Lipolotio	T156	5
Galderma / Noweda	Excipial [®] U Lipolotio	T073/170522EUL	1
Galderma / Phoenix	Excipial [®] U Lipolotio	363222	1
Galderma / SU	Excipial [®] U Lipolotio	375952	2
Galderma International	Excipial [®] U Lipolotio	354830	5
Galderma Internati...	Excipial [®] U Lipolotio	171711	4
Galderma Internati...	Excipial [®] U Lipolotio	173041	2
Galderma Labor.	Excipial [®] U Lipolotio	169110	6
Galderma Laborat. ...	Excipial [®] U Lipolotio	368867	1
Galderma Laborat. ...	Excipial [®] U Lipolotio	71415	1

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Supplier	Substance	Batch	Spectra
Galderma Laborator...	Excipial [®] U Lipolotio	368865	2
Galderma Laborator...	Excipial [®] U Lipolotio	375350	3
Galderma Laborator...	Excipial [®] U Lipolotio	380279	17
Galderma Laborator...	Excipial [®] U Lipolotio	377693	9
Galderma Laborator...	Excipial [®] U Lipolotio	350885	7
Galderma, Sanacorp	Excipial [®] U Lipolotio	L0TS042	1
Galderma/ Alliance	Excipial [®] U Lipolotio	T115	2
Galderma/ Fiebig	Excipial [®] U Lipolotio	830071/17	1
Galderma/ Noweda	Excipial [®] U Lipolotio	T072	1
Galderma/ Noweda	Excipial [®] U Lipolotio	L0T50450	2
Galderma/ Noweda	Excipial [®] U Lipolotio	312417	13
Galderma/ Noweda	Excipial [®] U Lipolotio	319844	8
Galderma/ NOWEDA	Excipial [®] U Lipolotio	V082	4
Galderma/AEP	Excipial [®] U Lipolotio	V165	2
Galderma/AHD	Excipial [®] U Lipolotio	323580	4
Galderma/AHD	Excipial [®] U Lipolotio	344636	10
Galderma/AHD	Excipial [®] U Lipolotio	351894	3
Galderma/Alliance	Excipial [®] U Lipolotio	T122	1
Galderma/Alliance	Excipial [®] U Lipolotio	S135	1
Galderma/Alliance ...	Excipial [®] U Lipolotio	T121	1
Galderma/anzag	Excipial [®] U Lipolotio	363069	2
Galderma/Anzag	Excipial [®] U Lipolotio	R183	1
Galderma/Anzag	Excipial [®] U Lipolotio	S206	2
Galderma/Fiebig	Excipial [®] U Lipolotio	V062	1
galderma/G	Excipial [®] U Lipolotio	L0TS202	1
Galderma/Galderma	Excipial [®] U Lipolotio	s017	1
Galderma/Galderma	Excipial [®] U Lipolotio	S017	1
Galderma/Galderma	Excipial [®] U Lipolotio	S142	1
Galderma/Galderma	Excipial [®] U Lipolotio	174960	1
Galderma/Gehe	Excipial [®] U Lipolotio	R189	1
Galderma/Gehe	Excipial [®] U Lipolotio	T061	3
Galderma/Gehe	Excipial [®] U Lipolotio	T066	1
Galderma/Gehe	Excipial [®] U Lipolotio	S139	1
Galderma/Gehe	Excipial [®] U Lipolotio	V108	2
Galderma/Gehe	Excipial [®] U Lipolotio	50691	3
Galderma/Gehe	Excipial [®] U Lipolotio	169831	1
Galderma/Gehe	Excipial [®] U Lipolotio	332540	9
Galderma/Gehe	Excipial [®] U Lipolotio	346461	1
Galderma/Gehe	Excipial [®] U Lipolotio	352411	4
Galderma/Gehe	Excipial [®] U Lipolotio	368866	3
Galderma/Jenne	Excipial [®] U Lipolotio	355167	4
Galderma/Kehr	Excipial [®] U Lipolotio	320973	6
Galderma/Noweda	Excipial [®] U Lipolotio	170420EUL/L0TS204	1
Galderma/Noweda	Excipial [®] U Lipolotio	170518EUL/L0TT073	1
Galderma/Noweda	Excipial [®] U Lipolotio	170316EL/L0TT073	1
Galderma/Noweda	Excipial [®] U Lipolotio	V041	6
Galderma/Noweda	Excipial [®] U Lipolotio	170906EL/T072	1
Galderma/Noweda	Excipial [®] U Lipolotio	50689	5
Galderma/Noweda	Excipial [®] U Lipolotio	50842	4
Galderma/Noweda	Excipial [®] U Lipolotio	319422	8
Galderma/Noweda	Excipial [®] U Lipolotio	330444	12
Galderma/Noweda	Excipial [®] U Lipolotio	326331	1
Galderma/Noweda	Excipial [®] U Lipolotio	342479	7
Galderma/Noweda	Excipial [®] U Lipolotio	363075	1
Galderma/phoen	Excipial [®] U Lipolotio	V166	1
Galderma/phoenix	Excipial [®] U Lipolotio	169847	1

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Supplier	Substance	Batch	Spectra
Galderma/Phoenix	Excipial [®] U Lipolotio	L0TT085	1
Galderma/Phoenix	Excipial [®] U Lipolotio	3717E-03749	1
Galderma/Phoenix	Excipial [®] U Lipolotio	V061	1
Galderma/Phoenix	Excipial [®] U Lipolotio	50450	3
Galderma/Phoenix	Excipial [®] U Lipolotio	175042	2
Galderma/Phonix	Excipial [®] U Lipolotio	V157	1
Galderma/phönix	Excipial [®] U Lipolotio	T091	2
Galderma/phönix	Excipial [®] U Lipolotio	V162	1
Galderma/Phönix	Excipial [®] U Lipolotio	T116	1
Galderma/Phönix	Excipial [®] U Lipolotio	V035	1
Galderma/Phönix	Excipial [®] U Lipolotio	V136	1
Galderma/Phönix	Excipial [®] U Lipolotio	50876	3
Galderma/Phönix	Excipial [®] U Lipolotio	170615	11
Galderma/Phönix	Excipial [®] U Lipolotio	170199	1
Galderma/Phönix	Excipial [®] U Lipolotio	170195	2
Galderma/Phönix	Excipial [®] U Lipolotio	174756	9
Galderma/Phönix	Excipial [®] U Lipolotio	171710	3
Galderma/Phönix	Excipial [®] U Lipolotio	173469	8
Galderma/Phönix	Excipial [®] U Lipolotio	174807	1
Galderma/Phönix	Excipial [®] U Lipolotio	309994	2
Galderma/Phönix	Excipial [®] U Lipolotio	335695	12
Galderma/Phönix	Excipial [®] U Lipolotio	358549	2
Galderma/Phönix	Excipial [®] U Lipolotio	371415	2
Galderma/S	Excipial [®] U Lipolotio	371412	6
Galderma/S	Excipial [®] U Lipolotio	369044	4
Galderma/sanacorp	Excipial [®] U Lipolotio	310709	15
Galderma/Sanacorp	Excipial [®] U Lipolotio	V073	1
Galderma/Sanacorp	Excipial [®] U Lipolotio	V103	2
Galderma/Sanacorp	Excipial [®] U Lipolotio	V151	1
Galderma/Sanacorp	Excipial [®] U Lipolotio	167638	2
Galderma/Sanacorp	Excipial [®] U Lipolotio	314142	7
Galderma/Spirig Ph. ...	Excipial [®] U Lipolotio	L0TR187	1
Galderma/Würmtal A...	Excipial [®] U Lipolotio	S132	3
Galderma/Würmtal- A...	Excipial [®] U Lipolotio	R142	1
Galderma/Würmtal- A...	Excipial [®] U Lipolotio	S071	5
Galderma/Würmtal- A...	Excipial [®] U Lipolotio	S205	2
Galderma/Würmtal- A...	Excipial [®] U Lipolotio	V142	1
Galderma/Sanacorp	Excipial [®] U Lipolotio	314603	9
Gehe	Excipial [®] U Lipolotio	S143	2
Gehe	Excipial [®] U Lipolotio	V152	3
Gehe	Excipial [®] U Lipolotio	V121	4
Gehe	Excipial [®] U Lipolotio	50688	3
Gehe	Excipial [®] U Lipolotio	V107	1
Gehe	Excipial [®] U Lipolotio	307766	2
Gehe	Excipial [®] U Lipolotio	332534	1
Gehe	Excipial [®] U Lipolotio	VT230419-0	2
Gehe	Excipial [®] U Lipolotio	354348	1
Gehe	Excipial [®] U Lipolotio	398081	2
GEHE	Excipial [®] U Lipolotio	50459	2
GEHE	Excipial [®] U Lipolotio	50890	3
GEHE	Excipial [®] U Lipolotio	174996	1
GEHE	Excipial [®] U Lipolotio	174966	5

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Supplier	Substance	Batch	Spectra
GEHE	Excipial [®] U Lipolotio	309197	3
GEHE	Excipial [®] U Lipolotio	312811	11
Gehe-Spring	Excipial [®] U Lipolotio	L0TR167	1
Caelo	Excipial [®] U Lipolotio	L0TS081	1
Gehe/Galderma	Excipial [®] U Lipolotio	LotV011	1
Kehr/Galderma	Excipial [®] U Lipolotio	T029	1
Nestle Skin Health	Excipial [®] U Lipolotio	318718	5
Nestle Skin Health...	Excipial [®] U Lipolotio	305489	13
Nestle Skin Health...	Excipial [®] U Lipolotio	303485	3
Nestle Skin Health...	Excipial [®] U Lipolotio	319344	1
Noweda	Excipial [®] U Lipolotio	R261	1
Noweda	Excipial [®] U Lipolotio	L0T50876	1
Caelo	Excipial [®] U Lipolotio	S203	2
Caelo	Excipial [®] U Lipolotio	50569	2
Phoenix	Excipial [®] U Lipolotio	N105	1
Phoenix	Excipial [®] U Lipolotio	S138	2
Phoenix	Excipial [®] U Lipolotio	S148	2
Phoenix	Excipial [®] U Lipolotio	319748	29
Phoenix / Bios Medical	Excipial [®] U Lipolotio	329498	1
Phoenix WE 16.01.1...	Excipial [®] U Lipolotio	L0TS122	2
Phoenix/Spirig	Excipial [®] U Lipolotio	N041	2
PHÖNIX	Excipial [®] U Lipolotio	T063	1
PHÖNIX	Excipial [®] U Lipolotio	V039	1
PHÖNIX	Excipial [®] U Lipolotio	V105	1
Sanacorp	Excipial [®] U Lipolotio	375946	3
sanacorp / Nestle	Excipial [®] U Lipolotio	174800	1
Caelo	Excipial [®] U Lipolotio	318628	5
spirig	Excipial [®] U Lipolotio	M142	1
spirig	Excipial [®] U Lipolotio	N013	1
spirig	Excipial [®] U Lipolotio	N061	2
spirig	Excipial [®] U Lipolotio	N058	4
spirig	Excipial [®] U Lipolotio	N086	2
spirig	Excipial [®] U Lipolotio	R037	1
Spirig	Excipial [®] U Lipolotio	M091	1
Spirig	Excipial [®] U Lipolotio	N123	1
Spirig	Excipial [®] U Lipolotio	R047	1
Spirig	Excipial [®] U Lipolotio	L0TT057	1
Spirig	Excipial [®] U Lipolotio	T149	3
Spirig	Excipial [®] U Lipolotio	169838	1
Spirig / Anzag	Excipial [®] U Lipolotio	N032	1
Spirig / Sanacorp	Excipial [®] U Lipolotio	R041	1
Spirig Pharma	Excipial [®] U Lipolotio	L0TK131	1
Spirig Pharma	Excipial [®] U Lipolotio	L0TN013	1
Spirig Pharma	Excipial [®] U Lipolotio	M134	1
Spirig Pharma	Excipial [®] U Lipolotio	S122	1
Spirig Pharma	Excipial [®] U Lipolotio	V053	4
Spirig Pharma	Excipial [®] U Lipolotio	V141	3
Spirig Pharma / Noweda	Excipial [®] U Lipolotio	S141	1
Spirig/ Noweda	Excipial [®] U Lipolotio	S225	1
Spirig/AHD	Excipial [®] U Lipolotio	M085	1
Spirig/AHD	Excipial [®] U Lipolotio	lotno86	1
Spirig/Galderma	Excipial [®] U Lipolotio	R156	2
Spirig/Galderma	Excipial [®] U Lipolotio	R146	1
Spirig/Gehe	Excipial [®] U Lipolotio	M102	2
Spirig/Gehe	Excipial [®] U Lipolotio	M146	1
Spirig/Gehe	Excipial [®] U Lipolotio	M182	2

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Supplier	Substance	Batch	Spectra
Spirig/Gehe	Excipial [®] U Lipolotio	R114	1
Spirig/Gehe	Excipial [®] U Lipolotio	R262	1
Spirig/Kehr	Excipial [®] U Lipolotio	V038	2
Spirig/Phönix	Excipial [®] U Lipolotio	R033	1
Spirig/Würmtal-Apotheke	Excipial [®] U Lipolotio	R145	2
Sprig (Galderma)/ G	Excipial [®] U Lipolotio	S123	2
	Excipial [®] U10 Lipolotio	375941	2
	Excipial [®] U10 Lipolotio	377695	1
	Excipial [®] U10 Lipolotio	382559	2
	Excipial [®] U10 Lipolotio	375353	1
	Excipial [®] U10 Lipolotio	388433	1
Galaderma/Krieger	Excipial [®] U10 Lipolotio	T071	1
Galderma	Excipial [®] U10 Lipolotio	V061	1
Galderma	Excipial [®] U10 Lipolotio	V096	1
Galderma	Excipial [®] U10 Lipolotio	L0T50679	1
Galderma	Excipial [®] U10 Lipolotio	169263	1
Galderma	Excipial [®] U10 Lipolotio	174117	1
Galderma	Excipial [®] U10 Lipolotio	304231	1
Galderma	Excipial [®] U10 Lipolotio	318218	1
Galderma	Excipial [®] U10 Lipolotio	15166	1
Galderma	Excipial [®] U10 Lipolotio	322729	2
Galderma/ Noweda	Excipial [®] U10 Lipolotio	50876	1
Galderma/AHCA	Excipial [®] U10 Lipolotio	L0T50604	1
Galderma/Alliance	Excipial [®] U10 Lipolotio	T042	1
Galderma/Alliance	Excipial [®] U10 Lipolotio	323868	2
Galderma/Galderma	Excipial [®] U10 Lipolotio	308310	4
Galderma/Gehe	Excipial [®] U10 Lipolotio	329100	1
Galderma/Krieger	Excipial [®] U10 Lipolotio	50581	3
Galderma/Phönix	Excipial [®] U10 Lipolotio	174116	1
Galderma/S	Excipial [®] U10 Lipolotio	347683	1
Galderma/Sanacorp	Excipial [®] U10 Lipolotio	V092	1
Galderma/Sanacorp	Excipial [®] U10 Lipolotio	50679	1
Galderma/Sanacorp	Excipial [®] U10 Lipolotio	169759	2
Galderma/Sanacorp	Excipial [®] U10 Lipolotio	308637	1
Galderma/Sanacorp	Excipial [®] U10 Lipolotio	308601	3
Galderma/Sanacorp	Excipial [®] U10 Lipolotio	320154	1
Galderma/Sanacorp	Excipial [®] U10 Lipolotio	321879	1
Galderma/Würmtal-Apo.	Excipial [®] U10 Lipolotio	T053	1
Galderma/Würmtal-A...	Excipial [®] U10 Lipolotio	V042	1
NesteSkin Health/gehe	Excipial [®] U10 Lipolotio	318209	3
Spirig Pharma AG	Excipial [®] U10 Lipolotio	V082	1
Spirig/AHD	Excipial [®] U10 Lipolotio	M025	1

F

Supplier	Substance	Batch	Spectra
Artesan	Fabitol [®] base cream	52003	6
	Fabitol [®] base cream	233421	2
	Fabitol [®] base cream	233332	1
	Fabitol [®] base cream	GLWW5	1
	Fabitol [®] base cream	glwd2	1
Caelo	Fabitol [®] base cream	GWWL3	1
Euro OTC	Fabitol [®] base cream	1016021	2
Fontapharm	Fabitol [®] base cream	GLWW4	1
Fontapharm	Fabitol [®] base cream	GLWD2	10

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Supplier	Substance	Batch	Spectra
Fontapharm	Fabitop [®] base cream	GLWD2x2	1
Fontapharm	Fabitop [®] base cream	GLWD5	5
Fontapharm	Fabitop [®] base cream	101601	18
Fontapharm / Phönix	Fabitop [®] base cream	1016022	4
Fontapharm / Phönix	Fabitop [®] base cream	101603	6
Fontapharm / Phönix	Fabitop [®] base cream	520012	2
Fontapharm/Gehe	Fabitop [®] base cream	GLWD4	2
Fontapharm/Gotha	Fabitop [®] base cream	520011	11
Fontapharm/Noweda	Fabitop [®] base cream	GLWD3	4
Fontapharm/phönix	Fabitop [®] base cream	52002	5
Gehe	Fabitop [®] base cream	GRWW2	7
jenne artesan	Fabitop [®] base cream	GLWWW5	1
Noweda	Fabitop [®] base cream	233511	1
Caelo	Fabitop [®] base cream	GWWL1	2
Fagron	Fitalite [™]	1503259	2

G

Supplier	Substance	Batch	Spectra
Gehe	Glycerol trinitrate 5%	214895	1
Gehe	Glycerol trinitrate 5%	221414	3
Pharmapohl	Glycerol trinitrate 5%	18102013A	1
Pharmapol	Glycerol trinitrate 5%	219108	4
Pharmapol	Glycerol trinitrate 5%	224310	5
Pharmapol	Glycerol trinitrate 5%	224310(ex)224658(in)	1
Pharmapol	Glycerol trinitrate 5%	226578	11
Pharmapol	Glycerol trinitrate 5%	228718	11
Pharmapol	Glycerol trinitrate 5%	25041301	1
Pharmapol	Glycerol trinitrate 5%	AKD81	1
Pharmapol	Glycerol trinitrate 5%	232961	3
Pharmapol	Glycerol trinitrate 5%	234783	2
Pharmapol	Glycerol trinitrate 5%	238259	1
Pharmapol Arzneimi...	Glycerol trinitrate 5%	232961	6
Pharmapol/Zentrum Apo	Glycerol trinitrate 5%	2913A-07002	1

H

Supplier	Substance	Batch	Spectra
	Hans Karrer Hydrocream Micr...	LOT22005	1
	Hans Karrer Hydrocream Micr...	22006	1
	Hans Karrer Hydrocream Micr...	23003	2
	Hans Karrer Hydrocream Micr...	23001	1
	Hans Karrer Hydrocream Micr...	23002	1
	Hans Karrer Hydrocream Micr...	23004	2
	Hans Karrer Hydrocream Micr...	LOT24002	3
	Hans Karrer Hydrocream Micr...	LOT23004	1
	Hans Karrer Hydrocream Micr...	24003	5
	Hans Karrer Hydrocream Micr...	LOT24003	1
	Hans Karrer Hydrocream Micr...	LOT24004	5
	Hans Karrer Hydrocream Micr...	24004	4
	Hans Karrer Hydrocream Micr...	LOT24005	2
	Hans Karrer Hydrocream Micr...	24005	1
	Hans Karrer Hydrocream Micr...	LOT25002MAR2028	1
	Hans Karrer Hydrocream Micr...	LOT25001	1
Hans Karrer	Hans Karrer Hydrocream Micr...	LOT20005	1
Hans Karrer	Hans Karrer Hydrocream Micr...	21001	2
Hans Karrer	Hans Karrer Hydrocream Micr...	21005	2
Hans Karrer / Anzag	Hans Karrer Hydrocream Micr...	18002	2

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Supplier	Substance	Batch	Spectra
Hans Karrer / Noweda	Hans Karrer Hydrocream Micr...	20007	1
Hans Karrer / Phönix	Hans Karrer Hydrocream Micr...	L0T20001	1
Hans Karrer GmbH	Hans Karrer Hydrocream Micr...	22002	2
Hans Karrer GmbH /...	Hans Karrer Hydrocream Micr...	18004	6
Hans Karrer GmbH /...	Hans Karrer Hydrocream Micr...	L0T21001	1
Hans Karrer GmbH /...	Hans Karrer Hydrocream Micr...	19002	3
Hans Karrer GmbH /...	Hans Karrer Hydrocream Micr...	200002	1
Hans Karrer/Phönix	Hans Karrer Hydrocream Micr...	20001	3
Hans Karrer/Phönix	Hans Karrer Hydrocream Micr...	20005	1
Hans Karrer/Sanacorp	Hans Karrer Hydrocream Micr...	21002	1
Hans Karrer/Sanacorp	Hans Karrer Hydrocream Micr...	21004	2
Hans-Karrer GmbH	Hans Karrer Hydrocream Micr...	18003	9
hanskarrer	Hans Karrer Hydrocream Micr...	19004	1
hanskarrer / Gehe	Hans Karrer Hydrocream Micr...	18001	2
HansKarrer/Krieger	Hans Karrer Hydrocream Micr...	19003	7
HansKarrerGmbH/Phoekd	Hans Karrer Hydrocream Micr...	20004	2
Karrer/Noweda	Hans Karrer Hydrocream Micr...	21003	4
Karrer/Phönix	Hans Karrer Hydrocream Micr...	19001	7
Noweda	Hans Karrer Hydrocream Micr...	L0T19001	2
Noweda	Hans Karrer Hydrocream Micr...	22005/2308293	1
Noweda	Hans Karrer Hydrocream Micr...	22002/2308232	1
	Hans Karrer Lipocream Micro...	24002	3
	Hans Karrer Lipocream Micro...	24003	1
Caelo	Hans Karrer Lipocream Micro...	L0T17001	1
hans karrer	Hans Karrer Lipocream Micro...	19005	1
Hans Karrer	Hans Karrer Lipocream Micro...	19001	1
Hans Karrer GmbH	Hans Karrer Lipocream Micro...	L0T20005	1
Hans Karrer/Sanac.	Hans Karrer Lipocream Micro...	21006	1
HansKarrer/Phoenix	Hans Karrer Lipocream Micro...	19004	1
Kirchstrasse	Hans Karrer Lipocream Micro...	17001	1
	Hans Karrer Lipolotion Micr...	21016	2
	Hans Karrer Lipolotion Micr...	22011	1
	Hans Karrer Lipolotion Micr...	23007	1
	Hans Karrer Lipolotion Micr...	23008	1
	Hans Karrer Lipolotion Micr...	24006	1
	Hans Karrer Lipolotion Micr...	24005	1
Caelo	Hans Karrer Lipolotion Micr...	L0T20001	1
Euro OTC	Hans Karrer Lipolotion Micr...	16010	1
Galderna/Phönix	Hans Karrer Lipolotion Micr...	20005	1
Hans Kaffer GmbH/ ...	Hans Karrer Lipolotion Micr...	21017	1
Hans Karrer	Hans Karrer Lipolotion Micr...	20003	2
Hans Karrer	Hans Karrer Lipolotion Micr...	21019	1
Hans Karrer / Anzag	Hans Karrer Lipolotion Micr...	16004	1
Hans Karrer GmbH	Hans Karrer Lipolotion Micr...	19011	2
Hans Karrer GmbH	Hans Karrer Lipolotion Micr...	20013	1
Hans Karrer GmbH/ ...	Hans Karrer Lipolotion Micr...	22003	3
Hans Karrer	Hans Karrer Lipolotion Micr...	L0T19009	1
GmbH/K...			
Hans Karrer/Alliance	Hans Karrer Lipolotion Micr...	17003	2
Hans Karrer/Alliance	Hans Karrer Lipolotion Micr...	17009	1
Hans Karrer/Gehe	Hans Karrer Lipolotion Micr...	17002	20
Hans Karrer/Noweda	Hans Karrer Lipolotion Micr...	21007	1
Hans Karrer/Phoe	Hans Karrer Lipolotion Micr...	17011	1
Hans Karrer/Phoe	Hans Karrer Lipolotion Micr...	L0T18005	1
hans karrer/phönix	Hans Karrer Lipolotion Micr...	18010	2
hanskarrer	Hans Karrer Lipolotion Micr...	L0T17005	1
hanskarrer	Hans Karrer Lipolotion Micr...	17005	2
hanskarrer	Hans Karrer Lipolotion Micr...	17007	2
hanskarrer	Hans Karrer Lipolotion Micr...	19009	1
HansKarrer/Phönix	Hans Karrer Lipolotion Micr...	19004	1

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Supplier	Substance	Batch	Spectra
HansKarrer/Phönix	Hans Karrer Lipolotion Micr...	21009	1
HansKarrer/Sanacorp	Hans Karrer Lipolotion Micr...	20007	4
HansKarrer/Sanacorp	Hans Karrer Lipolotion Micr...	LOT20007	1
KARRER/ E	Hans Karrer Lipolotion Micr...	LOT17002	1
KHA/Noweda	Hans Karrer Lipolotion Micr...	21008	1
Nowada	Hans Karrer Lipolotion Micr...	23007/2310240	1

K

Supplier	Substance	Batch	Spectra
Anzag/Galderma	Kerasal [®] base ointment	S075	1
Galderma/Gehe	Kerasal [®] base ointment	S061	1
Galderma/Anzag	Kerasal [®] base ointment	S041	4
Spirig	Kerasal [®] base ointment	LOTR012	1
Spirig Pharma	Kerasal [®] base ointment	N021	1
Spirig/Gehe	Kerasal [®] base ointment	S076	1
Spirig/Sanacorp	Kerasal [®] base ointment	N011	1

L

Supplier	Substance	Batch	Spectra
Gehe	La Roche-Posay Cold Cream N...	54M91P	2
La Roche-Posay	La Roche-Posay Cold Cream N...	54M11P	1
La Roche-Posay	La Roche-Posay Cold Cream N...	54M01P	1
Mea-SanacorpWE10.0...	La Roche-Posay Cold Cream N...	LOT54M91P	1
Caelo	La Roche-Posay Toleriane	54J500	1
Gehe	La Roche-Posay Toleriane	54P802	4
Roche Posay/Gehe	La Roche-Posay Toleriane	54R1011	1
Roche/AHD	La Roche-Posay Toleriane	54J800	1
dr.wolff/sanacorp	Linola [®] body milk	2280	1
Caelo	Linola [®] fat cream	435161	1
Caelo	Linola [®] fat cream	238540	2
Caelo	Linola [®] fat cream	438070	1
Caelo	Linola [®] fat cream	700320	2
Caelo	Linola [®] fat cream	803320	1
Dr wolff	Linola [®] fat cream	3330	1
Dr.	Linola [®] fat cream	438430	1
Dr. August Wolff GmbH	Linola [®] fat cream	807620	2
Dr. August Wolff GmbH	Linola [®] fat cream	807630	2
Dr. August Wolff GmbH	Linola [®] fat cream	901910	3
Dr. August Wolff GmbH	Linola [®] fat cream	909800	3
Dr. August Wolff GmbH	Linola [®] fat cream	909790	5
Dr. August Wolff GmbH	Linola [®] fat cream	909709	1
Dr. August Wolff GmbH	Linola [®] fat cream	140920	2
Dr. August Wolff G...	Linola [®] fat cream	6901	1
Dr. August Wolff	Linola [®] fat cream	902800	1
Wolff/Phönix			
Dr. Wolff	Linola [®] fat cream	237920	1
Dr. Wolff	Linola [®] fat cream	333650	1
Dr. Wolff	Linola [®] fat cream	432591	1
Dr. Wolff	Linola [®] fat cream	437270	1
Dr. Wolff	Linola [®] fat cream	438420	1
Dr. Wolff	Linola [®] fat cream	501020	1
Dr. Wolff	Linola [®] fat cream	505340	1
Dr. Wolff	Linola [®] fat cream	510480	2
Dr. Wolff	Linola [®] fat cream	702041	1
Dr. Wolff	Linola [®] fat cream	610320	1

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Supplier	Substance	Batch	Spectra
Dr. Wolff	Linola [®] fat cream	705555650	1
Dr. Wolff	Linola [®] fat cream	101808	1
Dr. Wolff	Linola [®] fat cream	907070	3
Dr. Wolff	Linola [®] fat cream	145110	1
Dr. Wolff / Allian...	Linola [®] fat cream	709800	1
Dr. Wolff / Gehe	Linola [®] fat cream	337860	1
Dr. Wolff / Anzag	Linola [®] fat cream	237710	1
Dr. Wolff 03.12.20...	Linola [®] fat cream	337701	1
Dr. Wolff/ Sanacorp	Linola [®] fat cream	3400	1
Dr. Wolff/Noweda	Linola [®] fat cream	1070	1
Dr. Wolff/Phönix	Linola [®] fat cream	700310	1
Dr. Wolff/Phönix	Linola [®] fat cream	810170	3
Dr. August Wolff Gm...	Linola [®] fat cream	710080	2
dr.wolff	Linola [®] fat cream	337760	2
dr.Wolff	Linola [®] fat cream	438440	3
Dr. Wolff	Linola [®] fat cream	431160	1
Dr. Wolff	Linola [®] fat cream	608210	1
Dr. Wolff	Linola [®] fat cream	810180	6
Dr. Wolff	Linola [®] fat cream	907080	5
Dr. Wolff	Linola [®] fat cream	6401	1
Dr. Wolff	Linola [®] fat cream	6410	2
Dr. Wolff	Linola [®] fat cream	143640	4
Dr. Wolff	Linola [®] fat cream	146820	3
Dr. Wolff - Noweda	Linola [®] fat cream	808280	1
Dr. Wolff/Alliance	Linola [®] fat cream	141780	1
Dr. Wolff/NOW	Linola [®] fat cream	435160	1
Dr. Wolff/Sanacorp	Linola [®] fat cream	704020	1
Gehe	Linola [®] fat cream	904651	2
Löwen City-Apothek...	Linola [®] fat cream	231060	1
Noweda	Linola [®] fat cream	902810	1
Noweda	Linola [®] fat cream	1720	1
Noweda	Linola [®] fat cream	3390	1
Noweda/Dr. wolff	Linola [®] fat cream	9550	1
Wolff	Linola [®] fat cream	608200	1
Wolff / Wolff	Linola [®] fat cream	431190	1
Wolff/Noweda	Linola [®] fat cream	704030	1
Wolff/Phöenix	Linola [®] fat cream	710060	1
Wolff/Phönix	Linola [®] fat cream	337770	2
Engel-Apotheke	Linola [®] H fat N	2319Q-07101	1
Caelo	Linola [®] O/W cream	1111111111	1
Caelo	Linola [®] O/W cream	239181	1
Caelo	Linola [®] O/W cream	238520	7
Caelo	Linola [®] O/W cream	238484	2
Caelo	Linola [®] O/W cream	330760	1
Caelo	Linola [®] O/W cream	438350	2
Caelo	Linola [®] O/W cream	236281	1
Caelo	Linola [®] O/W cream	238530	5
Chiesi	Linola [®] O/W cream	510792	2
chiesi / Noweda	Linola [®] O/W cream	331460	1
Dr Wolff/ Sanacorp	Linola [®] O/W cream	810150	2
Dr. August Wolff G...	Linola [®] O/W cream	144790	1
Dr. August Wolff G...	Linola [®] O/W cream	170522LC/701090	1
Dr. August Wolff G...	Linola [®] O/W cream	11680	1
Dr. August Wolff G...	Linola [®] O/W cream	808420	5
Dr. August Wolff G...	Linola [®] O/W cream	901150	9
Dr. August Wolff G...	Linola [®] O/W cream	908930	6

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Supplier	Substance	Batch	Spectra
Dr. August Wolff G...	Linola® O/W cream	904890	5
Dr. August Wolff G...	Linola® O/W cream	1750	1
Dr. August Wolff/S...	Linola® O/W cream	807360	2
Dr. August Wolff/S...	Linola® O/W cream	147340	5
Dr. Wolf/GEHE	Linola® O/W cream	437110	2
Dr. Wolff	Linola® O/W cream	233200	2
Dr. Wolff	Linola® O/W cream	431200	3
Dr. Wolff	Linola® O/W cream	435080	1
Dr. Wolff	Linola® O/W cream	432480	1
Dr. Wolff	Linola® O/W cream	435530	1
Dr. Wolff	Linola® O/W cream	434430	3
Dr. Wolff	Linola® O/W cream	437120	1
Dr. Wolff	Linola® O/W cream	438200	5
Dr. Wolff	Linola® O/W cream	505280	4
Dr. Wolff	Linola® O/W cream	504100	1
Dr. Wolff	Linola® O/W cream	508280	1
Dr. Wolff	Linola® O/W cream	505200	4
Dr. Wolff	Linola® O/W cream	512330	1
Dr. Wolff	Linola® O/W cream	602300	1
Dr. Wolff	Linola® O/W cream	602190	3
Dr. Wolff	Linola® O/W cream	605419	1
Dr. Wolff	Linola® O/W cream	605410	3
Dr. Wolff	Linola® O/W cream	606121	1
Dr. Wolff	Linola® O/W cream	904810	1
Dr. Wolff	Linola® O/W cream	5110	2
Dr. Wolff	Linola® O/W cream	145100	1
Dr. Wolff	Linola® O/W cream	147210	1
DR. WOLFF	Linola® O/W cream	234192	1
Dr. Wolff 25.03.2...	Linola® O/W cream	236290	4
Dr. Wolff / Sanacorp	Linola® O/W cream	338990	4
Dr. Wolff, Noweda	Linola® O/W cream	141820	1
Dr. Wolff/Gehe	Linola® O/W cream	138350	1
Dr. Wolff/Malteser	Linola® O/W cream	330751	1
Dr. Wolff/Malteser	Linola® O/W cream	333880	1
Dr. Wolff/Noweda	Linola® O/W cream	1090	3
Dr. August Wolff	Linola® O/W cream	233140	1
Dr. August Wolff	Linola® O/W cream	605560	1
Dr. August Wolff	Linola® O/W cream	505560	1
Dr. August Wolff Gm...	Linola® O/W cream	140350	1
Dr. August Wolff/Ebert	Linola® O/W cream	431250	1
Dr. August Wolff/Ebert	Linola® O/W cream	432970	1
Dr. August Wolff/Kehr	Linola® O/W cream	9525	2
Dr. Wolff	Linola® O/W cream	238482	1
Dr. Wolff	Linola® O/W cream	334003	1
Dr. Wolff	Linola® O/W cream	903600	5
Dr. Wolff	Linola® O/W cream	908380	5
Dr. Wolff	Linola® O/W cream	908630	2
Dr. Wolff	Linola® O/W cream	10520	3
Dr. Wolff	Linola® O/W cream	143610	1
Dr. Wolff	Linola® O/W cream	910420	5
DR. Wolff	Linola® O/W cream	1490	5
DR. Wolff	Linola® O/W cream	11410	3
Dr. Wolff / AHD	Linola® O/W cream	505020	1
Dr. Wolff/ Anzag	Linola® O/W cream	234193	1
Dr. Wolff/Fiebig	Linola® O/W cream	510430	3
Dr. Wolff/Fiebig	Linola® O/W cream	606120	1

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Supplier	Substance	Batch	Spectra
Dr. Wolff/Gehe	Linola [®] O/W cream	432490	3
Dr. Wolff/Gehe	Linola [®] O/W cream	438360	3
Dr. Wolff/Gehe	Linola [®] O/W cream	606100	4
Dr. Wolff/NOW	Linola [®] O/W cream	810780	2
Dr. Wolff/NOW	Linola [®] O/W cream	141250	9
Dr. Wolff/Noweda	Linola [®] O/W cream	905070	7
Dr. Wolff/Phoenix	Linola [®] O/W cream	904680	5
Dr. Wolz/Phönix	Linola [®] O/W cream	907050	2
Euro OTC	Linola [®] O/W cream	333730	1
Gehe	Linola [®] O/W cream	607140	3
Ichthyol/AHD	Linola [®] O/W cream		3
Noweda	Linola [®] O/W cream	90115	1
Noweda	Linola [®] O/W cream	3380	1
Noweda	Linola [®] O/W cream	7060	8
Phö/Dr. Wolff	Linola [®] O/W cream	901100	1
Phoenix/Wolff	Linola [®] O/W cream	333640	4
wolff	Linola [®] O/W cream	434320	3
Wolff	Linola [®] O/W cream	606110	1
Wolff / Gehe	Linola [®] O/W cream	431130	3
Wolff / Noweda	Linola [®] O/W cream	431120	4
Wolff GmbH/Sanacorp	Linola [®] O/W cream	903540	1
Wolff/Sanacorp	Linola [®] O/W cream	333630	2
Galderma	Lipoderm [®] lotion	50932	2
Galderma/Alliance	Lipoderm [®] lotion	L0TV012	2
Galderma/Alliance	Lipoderm [®] lotion	50316	2
Galderma/AllianceHC	Lipoderm [®] lotion	T011	4
Galderma/Kehr	Lipoderm [®] lotion	S021	6
Galderma/Noweda	Lipoderm [®] lotion	L0TV042	1
Galderma/Phoenix	Lipoderm [®] lotion	S041	5
Ichthyol/Phönix	Lipoderm [®] lotion	L0TT043	1
Noweda	Lipoderm [®] lotion	169310	7
spirig	Lipoderm [®] lotion	4622	1
Spirig	Lipoderm [®] lotion	R011	6
Spirig	Lipoderm [®] lotion	L0TR011	1
Spirig Pharma	Lipoderm [®] lotion	V012	1
Spirig Pharma AG	Lipoderm [®] lotion	N041	3
Spirig Pharma AG/A...	Lipoderm [®] lotion	N041	1
Spirig Pharma AG/A...	Lipoderm [®] lotion	R023	10
Spirig Pharma AG/A...	Lipoderm [®] lotion	R044	5
Spirig Pharma/Phoenix	Lipoderm [®] lotion	T043	3
Spirig/AHD	Lipoderm [®] lotion	L0TN041	1
Spirig/Phoenix	Lipoderm [®] lotion	M065	4
SpirigPharm/Noweda	Lipoderm [®] lotion	L0T50932	2
	Locobase [®] Protect	21CA1/75	1
	Locobase [®] Protect	21H64/75	1
	Locobase [®] Protect	22G60A	9
	Locobase [®] Protect	23F31B	1
	Locobase [®] Protect	24B58A	3
	Locobase [®] Protect	24I07B	4
	Locobase [®] Protect	24I107B	1
	Locobase [®] Protect	24I10B	3
	Locobase [®] Protect	24/07B	1
A.H.D.	Locobase [®] Protect	12/05/75	1
AHD	Locobase [®] Protect	13A18/76	1
Alfason/Gehe	Locobase [®] Protect	161J31/75	1
Alfason/krieger	Locobase [®] Protect	17F10/76	1

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Supplier	Substance	Batch	Spectra
Alliance Healthcare	Locobase [®] Protect	22H82A	8
anzag	Locobase [®] Protect	18I13/76	2
Astellas	Locobase [®] Protect	14c32-78	1
AStellas	Locobase [®] Protect	14J02/77	5
Astellas / Anzag	Locobase [®] Protect	15J3/79	1
Astellas / Noweda	Locobase [®] Protect	15D1179	1
Astellas / Noweda	Locobase [®] Protect	15J35/76	1
Astellas Pharma	Locobase [®] Protect	13K15/75	2
Astellas Pharma	Locobase [®] Protect	14C32/78	2
Astellas Pharma	Locobase [®] Protect	15D11/79	5
Astellas Pharma	Locobase [®] Protect	16A06/76	3
Astellas Pharma	Locobase [®] Protect	15J38/79	2
Astellas Pharma GmbH	Locobase [®] Protect	16H03/76	1
Astellas Pharma Gm...	Locobase [®] Protect	16D35/77	1
Astellas/Alliance	Locobase [®] Protect	16J31/75	1
Astellas/Gehe	Locobase [®] Protect	15B14/76	1
Astellas/Gehe	Locobase [®] Protect	16G03/75	1
Astellas/Gehe	Locobase [®] Protect	18H30/76	2
Astellas/Gehe	Locobase [®] Protect	19D87/75	4
Astellas/Sanacorp	Locobase [®] Protect	19D65/78	1
Caelo	Locobase [®] Protect	15J35/75	2
Caelo	Locobase [®] Protect	17EB/75	1
Caelo	Locobase [®] Protect	17017/76	1
Caeo/Noweda	Locobase [®] Protect	15H06/80	3
devesa/Phönix	Locobase [®] Protect	17F08/76	2
Ichtyol/Phönix	Locobase [®] Protect	13E08/75	2
Karo pharma	Locobase [®] Protect	21K41/77	2
Karo Pharma	Locobase [®] Protect	21C63/75	5
Karo Pharma / Anzag	Locobase [®] Protect	220216(22A11/76)	1
Karo Pharma AB/ Sa...	Locobase [®] Protect	22A11/76	6
Karo Pharma AB/ Sa...	Locobase [®] Protect	21A02/75	3
Karo Pharma GmbH	Locobase [®] Protect	21K4075	1
Karo Pharma/Alliance	Locobase [®] Protect	22B11A	1
Karo Pharma/Noweda	Locobase [®] Protect	20I48/79	1
Karo PhRMA	Locobase [®] Protect	22G44B	3
karoPharma/Gehe	Locobase [®] Protect	21K40/75	1
KaroPharma/Gehe	Locobase [®] Protect	20A13/75	3
KaroPharma/Sana	Locobase [®] Protect	21LD2/75	3
Kehr	Locobase [®] Protect	21CA1/76	1
leo	Locobase [®] Protect	19E10/75	1
Leo Pharma	Locobase [®] Protect	19D65/76	5
LEO Pharma	Locobase [®] Protect	17B27/75	1
LEO Pharma / Allia...	Locobase [®] Protect	17F20/76	1
LEO Pharma / Noweda	Locobase [®] Protect	17EB2/75	3
LEO Pharma / Noweda	Locobase [®] Protect	18D20/75(3x350g)	1
Leo Pharma/Gehe	Locobase [®] Protect	18F30/75	1
Leo/ Phönix	Locobase [®] Protect	17F46/76	2
LEO/Alliance Health-care	Locobase [®] Protect	18D19/76	2
Leo/Gehe	Locobase [®] Protect	17C17/76	1
Leo/Gehe	Locobase [®] Protect	17F44/76	1
Leo/Gehe	Locobase [®] Protect	18J36/75	2
Leo/Noweda	Locobase [®] Protect	18K01/77	1
Leo/Phönix	Locobase [®] Protect	18A29/75	2
Leopharm/AEP	Locobase [®] Protect	17EB3/75	2
Leopharm/Alliance hc	Locobase [®] Protect	18D20/75	7

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Supplier	Substance	Batch	Spectra
Noweda	Locobase [®] Protect	20J37/75	3
Noweda	Locobase [®] Protect	130225	1
Noweda-Astella	Locobase [®] Protect	15A01/79	1
Phönix	Locobase [®] Protect	19D88/75	4
Phönix	Locobase [®] Protect	20A14/75	9
Phönix	Locobase [®] Protect	23IN3A	2
Sanacorp	Locobase [®] Protect	12F23/76	1
Sanacorp	Locobase [®] Protect	13A16/76	2
Astellas	Locobase [®] Repair	13H02/76	1
Astellas	Locobase [®] Repair	15J09/75	2
GEHE	Locobase [®] Repair	17J11/79	1
GEHE	Locobase [®] Repair	17J13/76	1
GEHE	Locobase [®] Repair	17K83/75	1
GEHE	Locobase [®] Repair	18EB5/75	1
GEHE	Locobase [®] Repair	18I90/75	1
Karo Pharma/Noweda	Locobase [®] Repair	20F45/77	1
Karopharma/Noweda	Locobase [®] Repair	19DA8/75	1
LeoPharma /Noweda	A/S Locobase [®] Repair	18B26/76	1
LeoPharma /Noweda	A/S Locobase [®] Repair	18I88/75	1
LeoPharma /Noweda	A/S Locobase [®] Repair	19D05/75	1
Phoenix	Locobase [®] Repair	15/03/75	1
PHÖNIX	Locobase [®] Repair	17E81/75	2
PHÖNIX	Locobase [®] Repair	17E77/75	2
PHÖNIX	Locobase [®] Repair	17F72/75	1
Almirall	Lygal [®] head ointment N 3%	181908	1
Almirall	Lygal [®] head ointment N 3%	174928	1
Almirall mal/Noweda	Her- Lygal [®] head ointment N 3%	191407	1
Almirall/GEHE	Lygal [®] head ointment N 3%	174924	1
Almirall/GEHE	Lygal [®] head ointment N 3%	184027	2
Almirall/GEHE	Lygal [®] head ointment N 3%	184028	1
Almirall/GEHE	Lygal [®] head ointment N 3%	193815	1
Almirall/Otto	Lygal [®] head ointment N 3%	182913	1
Anzag/Gehe	Lygal [®] head ointment N 3%	202512	1
Caelo	Lygal [®] head ointment N 3%	181909	1
Fagron	Lygal [®] head ointment N 3%	181905	1
gehe	Lygal [®] head ointment N 3%	23060101/26	1
Sanacorp	Lygal [®] head ointment N 3%	223914	1
Taurus Pharma	Lygal [®] head ointment N 3%	134507	1
	Lygal [®] ointment base	214604	1
Allmirall	Lygal [®] ointment base	202504	16
Almiral / Gehe	Lygal [®] ointment base	175007	6
Almiral / Gehe	Lygal [®] ointment base	182905	2
Almirall	Lygal [®] ointment base	182002	1
Almirall	Lygal [®] ointment base	184607	2
Almirall	Lygal [®] ointment base	193202	4
Almirall	Lygal [®] ointment base	182904	10
Almirall	Lygal [®] ointment base	202102	3
Almirall	Lygal [®] ointment base	211301	1
almirall Hermal GmbH	Lygal [®] ointment base	192701	5
Almirall/ Gehe	Lygal [®] ointment base	175008	5
Almirall/GE-HH	Lygal [®] ointment base	202503	8
almirall/gehe	Lygal [®] ointment base	174106	5
Almirall/Gehe	Lygal [®] ointment base	182001	7

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Supplier	Substance	Batch	Spectra
Almirall/NOWEDA	Lygal [®] ointment base	214603	5
Almirall/Sanacorp	Lygal [®] ointment base	213602	4
Caelo	Lygal [®] ointment base	182903	7
Finteler Apotheke	Lygal [®] ointment base	1704011	2
Leyhs	Lygal [®] ointment base	202101	6
Phoenix WE: 08.11...	Lygal [®] ointment base	172803_2	2
TAUROS PHARMA	Lygal [®] ointment base	124803	3
TAUROS PHARMA	Lygal [®] ointment base	7.2016	1
TAUROS PHARMA	Lygal [®] ointment base	141601P	6
Taurus	Lygal [®] ointment base	133402	1
Taurus	Lygal [®] ointment base	141601T	1
Taurus	Lygal [®] ointment base	141603	2
Taurus	Lygal [®] ointment base	18121705	1
Taurus Pharma	Lygal [®] ointment base	133401T	6
Taurus Pharma	Lygal [®] ointment base	133401P	1
TAURUS PHARMA	Lygal [®] ointment base	141602T	1
Taurus Pharma GmbH	Lygal [®] ointment base	164803	1
Taurus Pharma/Jenne	Lygal [®] ointment base	1728031	1
Taurus/Alliance	Lygal [®] ointment base	1717022	2
Taurus/Alliance	Lygal [®] ointment base	1717021	1
Taurus/Phönix	Lygal [®] ointment base	154841	3

M

Supplier	Substance	Batch	Spectra
	Milk Cordes [®] O/W Emulsion	22D0014	10
	Milk Cordes [®] O/W Emulsion	22D0018	5
Caelo	Milk Cordes [®] O/W Emulsion	13D001	2
Ichthyol	Milk Cordes [®] O/W Emulsion	60613	1
Ichthyol - Gesellschaft	Milk Cordes [®] O/W Emulsion	11D037	1
Ichthyol / Noweda	Milk Cordes [®] O/W Emulsion	12D008	5
IchthyolGmbH/Anzag	Milk Cordes [®] O/W Emulsion	12D003	2
Ichthyol, Noweda	Milk Cordes [®] O/W Emulsion	13d007	1

N

Supplier	Substance	Batch	Spectra
	Neribas [®] cream	23A15A	1
	Neribas [®] cream	22A87776	1
	Neribas [®] cream	23E45A	4
	Neribas [®] cream	23G02A	2
	Neribas [®] cream	23602A	1
	Neribas [®] cream	23J95A	1
	Neribas [®] cream	24C53A	9
	Neribas [®] cream	24C08A	3
	Neribas [®] cream	24E02A	1
	Neribas [®] cream	24I24A	1
AHD	Neribas [®] cream	YY02804	2
AHD	Neribas [®] cream	YY0431K	8
Bayer/ Sanacorp	Neribas [®] cream	YY002L6	1
Caelo	Neribas [®] cream	yyo18ff	1
Caelo	Neribas [®] cream	YY01X64	1
Caelo	Neribas [®] cream	yy01kk7	1
Chiesi / Gehe	Neribas [®] cream	32097A	1
Euro OTC	Neribas [®] cream	YY02805	5
Caelo	Neribas [®] cream	yy01k94	1
Gehe	Neribas [®] cream	YY0167J	1

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Supplier	Substance	Batch	Spectra
Gehe	Neribas [®] cream	24K76A	5
Caelo	Neribas [®] cream	yy0203H	1
GP GmbH/Spangro	Neribas [®] cream	Y018FF	1
GP Grenzach Produkt...	Neribas [®] cream	YY01673	1
Intendis / Gehe	Neribas [®] cream	21076A	1
Intendis / Sanacorp	Neribas [®] cream	24105A	1
Intendis GmbH	Neribas [®] cream	24089A	1
Jena/Alliance	Neribas [®] cream	YY023J5	5
Jenapharm	Neribas [®] cream	33100C	1
Jenapharm	Neribas [®] cream	YY01K94	1
Jenapharm	Neribas [®] cream	YY0277H	1
Jenapharm / Gehe	Neribas [®] cream	34104C	1
Jenapharm / Noweda	Neribas [®] cream	YY00C34	1
Jenapharm/	Neribas [®] cream	YY005HT	3
Jenapharm/	Neribas [®] cream	YY01KK7	3
Jenapharm/ Noweda	Neribas [®] cream	YY00216	1
Jenapharm/ Noweda	Neribas [®] cream	YY01TCN	1
Jenapharm/Alliance	Neribas [®] cream	YY000C3	2
Jenapharm/Alliance	Neribas [®] cream	YY001HS	1
Jenapharm/Alliance	Neribas [®] cream	YY006LX	1
Jenapharm/Krieger	Neribas [®] cream	YY02H20	9
Jenapharm/Noweda	Neribas [®] cream	YY00C35	2
Jenapharm/Noweda	Neribas [®] cream	YY00XEF	2
Jenapharm/Noweda	Neribas [®] cream	YY014NJ	2
Jenapharm/Noweda	Neribas [®] cream	YY01CXP	2
Jenapharm/Phokd	Neribas [®] cream	YY0203H	5
Jenapharm/Sanacorp	Neribas [®] cream	YY02L84	8
karo	Neribas [®] cream	yy052e2	1
KARO	Neribas [®] cream	22a88/75	1
Karo Pharm	Neribas [®] cream	22AB87/75	1
Karo Pharm AB /	Neribas [®] cream	YY04L5T	2
Phoenix			
Karo Pharma	Neribas [®] cream	YY04F1K	1
KARO Pharma	Neribas [®] cream	YY04P2E	7
KARO PHARMA	Neribas [®] cream	YY04EYL	12
Karo Pharma / Gehe	Neribas [®] cream	22A87/75	2
Karo Pharma GmbH	Neribas [®] cream	22A88/75	6
Karo/Jenne	Neribas [®] cream	YY04FEK	2
Karo/Jenne	Neribas [®] cream	YY04FEL	2
Karo/Jenne	Neribas [®] cream	YY052E1	14
Karo/Jenne	Neribas [®] cream	YY052E2	9
Krieger	Neribas [®] cream	3388	1
Leo Pharma	Neribas [®] cream	yy0431j	1
Leo Pharma	Neribas [®] cream	yy0431ik	4
Leo Pharma	Neribas [®] cream	yy04EYL	1
LEO/Jenne	Neribas [®] cream	YY043TY	3
Leopharm	Neribas [®] cream	YY02TTH	7
Neribas	Neribas [®] cream	YY006KY	2
Noweda	Neribas [®] cream	YY04FEJ	5
Noweda	Neribas [®] cream	22A87/75/2308292	1
Noweda	Neribas [®] cream	23E45A/2310250	2
Noweda	Neribas [®] cream	22A8875/2311240	1
Noweda	Neribas [®] cream	24C08A/2407250	1
Noweda	Neribas [®] cream	24C53A/2410220	1
Noweda	Neribas [®] cream	24053A	1
Noweda	Neribas [®] cream	24E02A/2503130	1

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Supplier	Substance	Batch	Spectra
Caelo	Neribas [®] cream	yy02805	2
Noweda/Jenapharm	Neribas [®] cream	YY00PF1	1
Phoenix	Neribas [®] cream	3094	1
Phoenix	Neribas [®] cream	3229	1
Phoenix	Neribas [®] cream	3378	1
Phoenix	Neribas [®] cream	YY08H20	1
Phönix	Neribas [®] cream	3139	1
Phönix / Jenapharm	Neribas [®] cream	YY01FX3	1
Sanacorp	Neribas [®] cream	YY0431J	7
Sanacorp	Neribas [®] cream	22A87/75/2310041	1
	Neribas [®] fat ointment	23IS8A	3
	Neribas [®] fat ointment	24B24A	3
	Neribas [®] fat ointment	6696045	1
/ AHD	Neribas [®] fat ointment	YY016LP	4
BAYER/Phönix	Neribas [®] fat ointment	YY011K0	1
WE:26...			
Caelo	Neribas [®] fat ointment	yy00k7C	1
Elbdeich Apotheke ...	Neribas [®] fat ointment	YY04f1L	1
Jenapharm / Fiebig	Neribas [®] fat ointment	YY01TF2	6
Jenapharm/	Neribas [®] fat ointment	YY011K0	1
Jenapharm/Ahd	Neribas [®] fat ointment	YYo11Ko	1
Jenapharm/Gehe	Neribas [®] fat ointment	YY01PFP	1
Jenapharm/Phönix	Neribas [®] fat ointment	YY00K7C	1
Jenapharm/Phönix	Neribas [®] fat ointment	YY0282F	13
Karo Pharma	Neribas [®] fat ointment	22AB1/75	1
Karo Pharma/ Gehe	Neribas [®] fat ointment	YY04F1L	15
Karo Pharma/ Gehe	Neribas [®] fat ointment	YY04P2K	8
Karo Pharma/ Gehe	Neribas [®] fat ointment	YYo4P2K	1
Karo Pharma/ sanacorp	Neribas [®] fat ointment	YY054E8	5
leo Pharma	Neribas [®] fat ointment	yy0431T	1
LEO Pharma A/S	Neribas [®] fat ointment	YY04311	1
LeoPharma/Phönix	Neribas [®] fat ointment	YY0431T	10
Noweda	Neribas [®] fat ointment	YY02L7L	8
Noweda	Neribas [®] fat ointment	YY02L7L	1
Phoenix	Neribas [®] fat ointment	YY00K7C	2
Phoenix WE 24.04.1...	Neribas [®] fat ointment	YY019KR	1
	Neribas [®] ointment	230505 (YY0577C)	1
	Neribas [®] ointment	22K06A	10
	Neribas [®] ointment	220623 (Y0577C)	1
	Neribas [®] ointment	22K06a	1
	Neribas [®] ointment	231002 (22K06A)	1
	Neribas [®] ointment	23E46A	13
	Neribas [®] ointment	23H33A	6
	Neribas [®] ointment	23H34B	3
	Neribas [®] ointment	24BN4A	8
	Neribas [®] ointment	240909 (24BN4A)	1
	Neribas [®] ointment	24bn4a	1
	Neribas [®] ointment	250319 (24K91B)	1
	Neribas [®] ointment	24K91B	2
	Neribas [®] ointment	24K90A	10
	Neribas [®] ointment	24KS0A	1
	Neribas [®] ointment	34K91B	1
	Neribas [®] ointment	6697144	4
AHD	Neribas [®] ointment	22K06A	1
Anzag	Neribas [®] ointment	230810 (YY0577C)	1
Anzag	Neribas [®] ointment	231207 (23E46A)	1

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Supplier	Substance	Batch	Spectra
Anzag	Neribas [®] ointment	240117 (23E46A)	1
Anzag	Neribas [®] ointment	240226 (23E46A)	1
Anzag	Neribas [®] ointment	240416 (23H33A)	1
Anzag	Neribas [®] ointment	240522 (23H33A)	1
Anzag	Neribas [®] ointment	240730 (24BN4A)	1
Anzag	Neribas [®] ointment	240820 (24BN4A)	1
Anzag	Neribas [®] ointment	241021 (24BN4A)	1
Anzag	Neribas [®] ointment	241203 (24BN4A)	1
Anzag	Neribas [®] ointment	250109 (24BN4A)	1
Anzag	Neribas [®] ointment	250522 (24K90A)	1
Bayer/ Sanacorp	Neribas [®] ointment	YY006JT	5
Caelo	Neribas [®] ointment	YY00TJ0	2
Caelo	Neribas [®] ointment	YY00CC8	1
Jenaparm	Neribas [®] ointment	12091812	1
Jenapharm	Neribas [®] ointment	YY00K7E	3
Jenapharm	Neribas [®] ointment	YY011KX	1
Jenapharm	Neribas [®] ointment	YY016LN	3
Jenapharm	Neribas [®] ointment	YY017LF	1
Jenapharm	Neribas [®] ointment	YY01FX4	7
Jenapharm	Neribas [®] ointment	YY01KHH	4
Jenapharm	Neribas [®] ointment	YY023JE	6
Jenapharm	Neribas [®] ointment	YY023J1	2
Jenapharm	Neribas [®] ointment	5121811	1
Jenapharm	Neribas [®] ointment	YY02825	11
Jenapharm / Anzag	Neribas [®] ointment	YY00THL	8
Jenapharm / Anzag	Neribas [®] ointment	75 (YY02825)	1
Jenapharm / Anzag	Neribas [®] ointment	76 (YY02825)	1
Jenapharm / Anzag	Neribas [®] ointment	80 (YY02L27)	1
Jenapharm / Anzag	Neribas [®] ointment	84 (YY02L88)	1
Jenapharm / Anzag	Neribas [®] ointment	85 (YY02L88)	1
Jenapharm / Anzag	Neribas [®] ointment	88 (YY02L88)	1
Jenapharm / Anzag	Neribas [®] ointment	89 (YY02L88)	1
Jenapharm Anzag	Neribas [®] ointment	70 (YY01YEX)	1
Jenapharm Anzag	Neribas [®] ointment	71 (YY023J1)	1
Jenapharm Anzag	Neribas [®] ointment	72 (YY02835)	1
Jenapharm Anzag	Neribas [®] ointment	81 (YY02L27)	1
Jenapharm Anzag	Neribas [®] ointment	82 (YY02L88)	1
Jenapharm Anzag	Neribas [®] ointment	83 (YY02L88)	1
Jenapharm Anzag	Neribas [®] ointment		1
Jenapharm GmbH	Neribas [®] ointment	YY019PE	1
Jenapharm/ Anzag	Neribas [®] ointment	77 (YY02825)	1
Jenapharm/ Anzag	Neribas [®] ointment	78 (YY02L27)	1
Jenapharm/ Anzag	Neribas [®] ointment	79 (YY02L27)	1
Jenapharm/ Anzag	Neribas [®] ointment	86 (YY02L88)	1
Jenapharm/ Gehe	Neribas [®] ointment	YY02L27	2
Jenapharm/ Sanacorp	Neribas [®] ointment	YY01TF3	5
Jenapharm/AHD	Neribas [®] ointment	42 (YY011KX)	1
Jenapharm/AHD	Neribas [®] ointment	43 (YY00TJ0)	1
Jenapharm/AHD	Neribas [®] ointment	44 (YY011KX)	1
Jenapharm/AHD	Neribas [®] ointment	45 (YY017LF)	1
Jenapharm/AHD	Neribas [®] ointment	42 (YY016LN)	1
Jenapharm/AHD	Neribas [®] ointment	43 (YY016LN)	1
Jenapharm/AHD	Neribas [®] ointment	48 (144YY017LF)	1
Jenapharm/AHD	Neribas [®] ointment	49 (YY016EC)	1
Jenapharm/AHD	Neribas [®] ointment	50 (YY017LF)	1
Jenapharm/AHD	Neribas [®] ointment	51 (YY016EC)	1

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Supplier	Substance	Batch	Spectra
Jenapharm/AHD	Neribas [®] ointment	52(YY016EC)	1
Jenapharm/AHD	Neribas [®] ointment	53(YY01FX4)	1
Jenapharm/AHD	Neribas [®] ointment	54(YY0180C)	1
Jenapharm/AHD	Neribas [®] ointment	55(YY01FX4)	1
Jenapharm/AHD	Neribas [®] ointment	56(YY01FX4)	1
Jenapharm/AHD	Neribas [®] ointment	57(YY01FX4)	1
Jenapharm/AHD	Neribas [®] ointment	58(YY0180C)	1
Jenapharm/AHD	Neribas [®] ointment	58(YY01FX4)	1
Jenapharm/AHD	Neribas [®] ointment	59(YY01KHH)	1
Jenapharm/AHD	Neribas [®] ointment	60(YY01KHH)	2
Jenapharm/AHD	Neribas [®] ointment	61(YY01KHH)	1
Jenapharm/AHD	Neribas [®] ointment	62(YY01KHH)	1
Jenapharm/AHD	Neribas [®] ointment	65(YY019PE)	1
Jenapharm/AHD	Neribas [®] ointment	66(YY01TF3)	1
Jenapharm/AHD	Neribas [®] ointment	67(YY01TF3)	1
Jenapharm/AHD	Neribas [®] ointment	68(YY01YEX)	1
Jenapharm/Alliance	Neribas [®] ointment	YY016EC	3
Jenapharm/Anzag	Neribas [®] ointment	YY00XEH	4
Jenapharm/Anzag	Neribas [®] ointment	69(YY01YEX)	1
Jenapharm/Gehe	Neribas [®] ointment	YY01YEX	1
Jenapharm/Jenne	Neribas [®] ointment	61(YY019PE)	1
Jenapharm/Sanacorp	Neribas [®] ointment	YY0180C	1
Jenne	Neribas [®] ointment	230328(YY0577C)	1
Karo / A	Neribas [®] ointment	YY0577C	10
Karo Pharma	Neribas [®] ointment	YY04F1P	5
Karo Pharma	Neribas [®] ointment	22B10/78	3
Karo Pharma / Anzag	Neribas [®] ointment	99(YY04F1P)	1
Karo Pharma / Anzag	Neribas [®] ointment	100(YY04F1P)	1
Karo Pharma / Anzag	Neribas [®] ointment	101(YY04F1P)	1
Karo Pharma / Anzag	Neribas [®] ointment	102(YY04F1P)	1
Karo Pharma / Anzag	Neribas [®] ointment	103(YY04KYC)	1
Karo Pharma / Anzag	Neribas [®] ointment	104(YY04KYC)	1
Karo Pharma / Anzag	Neribas [®] ointment	211227(YY051T6)	1
Karo Pharma / Anzag	Neribas [®] ointment	220110(YY051T6)	1
Karo Pharma / Anzag	Neribas [®] ointment	220323(YY051T5)	1
Karo Pharma / Anzag	Neribas [®] ointment	220323(YY051T6)	1
Karo Pharma / Anzag	Neribas [®] ointment	220323(YY04T3L)	1
Karo Pharma / Anzag	Neribas [®] ointment	220721(YY0577C)	1
Karo Pharma / Anzag	Neribas [®] ointment	221122(YY0577C)	1
Karo Pharma / Anzag	Neribas [®] ointment	230202(22B10/78)	1
Karo Pharma / Anzag	Neribas [®] ointment	230309(22B10/78)	1
Karo Pharma / Jenne	Neribas [®] ointment	98(YY04F1P)	1
Karo Pharma / Jenne	Neribas [®] ointment	220518(YY0577C)	1
Karo Pharma GmbH	Neribas [®] ointment	22B09/78	3
Karo/ Jenne	Neribas [®] ointment	YY051T5	10
Karo/Jenne	Neribas [®] ointment	YY051t5	1
Leo Pharma A/S	Neribas [®] ointment	YY0431Y	3
Leo Pharma/ Anzag	Neribas [®] ointment	90(YY0431X)	1
Leo Pharma/ Anzag	Neribas [®] ointment	91(YY0431X)	1
Leo Pharma/ Anzag	Neribas [®] ointment	92(YY0431X)	1
Leo Pharma/ Anzag	Neribas [®] ointment	93(YY0431Y)	1
Leo Pharma/ Anzag	Neribas [®] ointment	94(YY0431Y)	1
Leo Pharma/ Anzag	Neribas [®] ointment	95(YY0431Y)	1
Leo Pharma/ Gehe	Neribas [®] ointment	YY04KYC	5
Leo Pharma/ Jenne	Neribas [®] ointment	96(YY0431Y)	1
Leo Pharma/ Jenne	Neribas [®] ointment	97(YY0431Y)	1

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Supplier	Substance	Batch	Spectra
Leo/ Jenne	Neribas [®] ointment	YY04T3L	4
Leopharma/Jenne	Neribas [®] ointment	YY02L88	12
Neribas Salbe	Neribas [®] ointment	YY051T6	3
Phoenix / Karo Pharma	Neribas [®] ointment	yy04Kyc	1
Phönix	Neribas [®] ointment	YY0431X	1
Phönix	Neribas [®] ointment	s.Zertifikat	1
Phönix	Neribas [®] ointment	YY0431x	1
Römer/apo	Neribas [®] ointment	YY008RJ	1
Wolf Apotheke	Neribas [®] ointment	73(YY02825)	1
Wolf Apotheke	Neribas [®] ointment	74(YY02825)	1
	Neuroderm [®] moisturising cream	S102214.1	2
	Neuroderm [®] moisturising cream	S052209.1	1
	Neuroderm [®] moisturising cream	S022302.1	1
	Neuroderm [®] moisturising cream	S102216.1	2
	Neuroderm [®] moisturising cream	S102211.1	2
	Neuroderm [®] moisturising cream	S022307.1	2
	Neuroderm [®] moisturising cream	S102212.1	1
	Neuroderm [®] moisturising cream	S022306.1	1
	Neuroderm [®] moisturising cream	S022309.1	4
	Neuroderm [®] moisturising cream	S022303.1	1
	Neuroderm [®] moisturising cream	S022304.1	2
	Neuroderm [®] moisturising cream	S062311.1	3
	Neuroderm [®] moisturising cream	S092316.1	2
	Neuroderm [®] moisturising cream	S062312.1	1
	Neuroderm [®] moisturising cream	S092317.1	2
	Neuroderm [®] moisturising cream	S122320.1	1
	Neuroderm [®] moisturising cream	S0824021	1
	Neuroderm [®] moisturising cream	S122322.1	1
	Neuroderm [®] moisturising cream	S012401.1	1
	Neuroderm [®] moisturising cream	S112408.1	1
	Neuroderm [®] moisturising cream	S082404.1	1
Alliance Healthcare	Neuroderm [®] moisturising cream	S101909.1	1
Caelo	Neuroderm [®] moisturising cream	V011704.1	1
Caelo	Neuroderm [®] moisturising cream	S071716.1	4
Caelo	Neuroderm [®] moisturising cream	6051801	1
Caelo	Neuroderm [®] moisturising cream	S221041	1
Caelo	Neuroderm [®] moisturising cream	S081618.1	1
Caelo	Neuroderm [®] moisturising cream	S071715.1	1
gehe	Neuroderm [®] moisturising cream	S102213.1	2
HÄLSA Pharma GmbH	Neuroderm [®] moisturising cream	S081518.1	1
...			
Infecto Pharm	Neuroderm [®] moisturising cream	V012002.1	1
Infecto/Phönix	Neuroderm [®] moisturising cream	S121731.1	1
infectopharm	Neuroderm [®] moisturising cream	S021310.1	1
Infectopharm	Neuroderm [®] moisturising cream	S071318.1	1
Infectopharm	Neuroderm [®] moisturising cream	S101325.1	1
Infectopharm	Neuroderm [®] moisturising cream	S031410.1	1
Infectopharm	Neuroderm [®] moisturising cream	S101429.1	2
Infectopharm	Neuroderm [®] moisturising cream	S121523.1	1
Infectopharm	Neuroderm [®] moisturising cream	S021609.1	1
Infectopharm	Neuroderm [®] moisturising cream	S022105.1	2
InfectoPharm	Neuroderm [®] moisturising cream	S021708.1	1
InfectoPharm	Neuroderm [®] moisturising cream	S071716.1	1
InfectoPharm	Neuroderm [®] moisturising cream	S071717.1	1
InfectoPharm	Neuroderm [®] moisturising cream	S121725.1	1
InfectoPharm	Neuroderm [®] moisturising cream	s071716.1	1

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Supplier	Substance	Batch	Spectra
InfectoPharm	Neuroderm [®] moisturising cream	S121733.1	3
InfectoPharm	Neuroderm [®] moisturising cream	9051801.1	1
InfectoPharm	Neuroderm [®] moisturising cream	S101807.1	3
InfectoPharm	Neuroderm [®] moisturising cream	S031902.1	2
InfectoPharm	Neuroderm [®] moisturising cream	S101910.1	1
InfectoPharm	Neuroderm [®] moisturising cream	S101908.1	1
InfectoPharm	Neuroderm [®] moisturising cream	S102008.1	1
InfectoPharm	Neuroderm [®] moisturising cream	S092109.1	3
InfectoPharm	Neuroderm [®] moisturising cream	S102214	1
InfectoPharm / Phoenix	Neuroderm [®] moisturising cream	S012203.1	1
InfectoPharm / Phoenix	Neuroderm [®] moisturising cream	S102210.1	4
InfectoPharm /AEP	Neuroderm [®] moisturising cream	S061514.1	2
Infectopharm, Noweda	Neuroderm [®] moisturising cream	S121726.1	1
infectopharm,Gehe	Neuroderm [®] moisturising cream	V011702.1	1
InfectoPharm/ Gehe	Neuroderm [®] moisturising cream	S112116.1	2
Infectopharm/AHD	Neuroderm [®] moisturising cream	S031904.1	1
Infectopharm/AHD	Neuroderm [®] moisturising cream	S031905.1	1
Infectopharm/AHD	Neuroderm [®] moisturising cream	S072002.1	1
Infectopharm/Alliance	Neuroderm [®] moisturising cream	S081616.1	1
Infectopharm/Alliance	Neuroderm [®] moisturising cream	S111631.1	1
Infectopharm/Alliance	Neuroderm [®] moisturising cream	S051803.1	1
Infectopharm/Fiebig	Neuroderm [®] moisturising cream	S081625.1	1
Infectopharm/Gehe	Neuroderm [®] moisturising cream	S0315081	1
Infectopharm/Gehe	Neuroderm [®] moisturising cream	V012001.1	5
Infectopharm/Gehe	Neuroderm [®] moisturising cream	S102007.1	2
Infectopharm/Gehe	Neuroderm [®] moisturising cream	S112118.1.1	1
Infectopharm/Gehe	Neuroderm [®] moisturising cream	S112118.1.1.	1
Infectopharm/Gehe	Neuroderm [®] moisturising cream	S042207.1	2
InfectoPharm/Gehe	Neuroderm [®] moisturising cream	S042206.01	1
InfectoPharm/Gehe	Neuroderm [®] moisturising cream	S112118.1	1
Infectopharm/Kehr	Neuroderm [®] moisturising cream	S031408.1	1
Infectopharm/Noweda	Neuroderm [®] moisturising cream	AS051801.1	2
Infectopharm/Noweda	Neuroderm [®] moisturising cream	V021903.1	2
Infectopharm/Noweda	Neuroderm [®] moisturising cream	S092107.1	2
InfectoPharm/Noweda	Neuroderm [®] moisturising cream	S102006.1	2
InfectoPharm/Noweda	Neuroderm [®] moisturising cream	S022102.1	1
InfectoPharm/Noweda	Neuroderm [®] moisturising cream	S022101.1	1
InfectoPharm/Noweda	Neuroderm [®] moisturising cream	S092110.1	1
Infectopharm/Phoenix	Neuroderm [®] moisturising cream	V012002.1	1
Infectopharm/Phönix	Neuroderm [®] moisturising cream	S021702.1	1
Infectopharm/Phönix	Neuroderm [®] moisturising cream	S021705.1	1
Infectopharm/Phönix	Neuroderm [®] moisturising cream	S071712.1	1
Infectopharm/Phönix	Neuroderm [®] moisturising cream	S101722.1	1
Infectopharm/Phönix	Neuroderm [®] moisturising cream	S1101724.1	1
Infectopharm/Phönix	Neuroderm [®] moisturising cream	S101724.1	3
Infectopharm/Phönix	Neuroderm [®] moisturising cream	S121732.1	1
Infectopharm/Phönix	Neuroderm [®] moisturising cream	V112005.1	1
Infectopharm/Phönix	Neuroderm [®] moisturising cream	S112117.1	1
InfectoPharma/Alli...	Neuroderm [®] moisturising cream	S121730.1	1
Infetopharm	Neuroderm [®] moisturising cream	S051802.1	1
Noweda	Neuroderm [®] moisturising cream	S071417.2	1
Noweda	Neuroderm [®] moisturising cream	V021902.1	2
Bombastus	Neuroderm [®] moisturising cream	S071412.1	1
PHÖNIX	Neuroderm [®] moisturising cream	S021703.1	2
Sanacorp	Neuroderm [®] moisturising cream	S021302.1	1
Sanacorp	Neuroderm [®] moisturising cream	s061514.1	1

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Supplier	Substance	Batch	Spectra
Infectopharm	Neuroderm [®] moisturising cre. ...		1
Infectopharm/AHD	Neuroderm [®] moisturising cre. ...	S021301.1	1

O

Supplier	Substance	Batch	Spectra
Almirall/Gehe	Optiderm [®] lotion	108201	1
Fagron	Ora-Blend [®] SF	3745164	1
Fagron	Ora-Blend [®] SF	4136370	1
Gehe	Ora-Blend [®] SF	2038178	1
Gehe	Ora-Blend [®] SF	3112578	1
Perrigo	Ora-Blend [®] SF	2088609	1
Phönix	Ora-Blend [®] SF	3434856	2
Phönix	Ora-Blend [®] SF	3475164	1
Fagron	Ora-Sweet [®]	3414679	1
Fagron	Ora-Sweet [®]	4247427	2

P

Supplier	Substance	Batch	Spectra
Caelo	Perfume oil vanilla	15316308	12
Caelo	Perfume oil vanilla	17054404	3
GSK Stiefel	Physiogel [®] hypoallergenic cream	859R	1
GSK/Stiefel	Physiogel [®] hypoallergenic cream	538T	1
PHOENIX 21.10.2013	Physiogel [®] hypoallergenic cream	1142N	1
Phoenix/Stiefel	Physiogel [®] hypoallergenic cream	399P	1
Stiefel	Physiogel [®] hypoallergenic cream	926Q	1
Stiefel	Physiogel [®] hypoallergenic cream	270T	1
Stiefel	Physiogel [®] hypoallergenic cream	537T	1
Stiefel/Noweda	Physiogel [®] hypoallergenic cream	163R	1
Stiefel/Sanacorp	Physiogel [®] hypoallergenic cream	10000	1
	Protegin [®] XN	22000510011	3
	Protegin [®] XN	23001097004	4
	Protegin [®] XN	23001097005	5
	Protegin [®] XN	23002995001	3
	Protegin [®] XN	23001097007	3
	Protegin [®] XN	23002995003	3
	Protegin [®] XN	23002995007	6
	Protegin [®] XN	24001198004	1
	Protegin [®] XN	24001198002	4
-	Protegin [®] XN	2711E-03598	1
22000510003	Protegin [®] XN	22000510003	2
Caelo	Protegin [®] XN	3091208	1
Caelo	Protegin [®] XN	11196702	2
Caelo	Protegin [®] XN	11022403	1
Caelo	Protegin [®] XN	12229201	6
Caelo	Protegin [®] XN	11196802	1
Caelo	Protegin [®] XN	8031305	1
Caelo	Protegin [®] XN	12229211	6
Caelo	Protegin [®] XN	12229210	2
Caelo	Protegin [®] XN	25061301	1
Caelo	Protegin [®] XN	12229209	1
Caelo	Protegin [®] XN	13081903	1
Caelo	Protegin [®] XN	13081908	1
Caelo	Protegin [®] XN	6012014A	1
Caelo	Protegin [®] XN	20011402	1
Caelo	Protegin [®] XN	13081904	2

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Supplier	Substance	Batch	Spectra
Caelo	Protegin [®] XN	13091906	1
Caelo	Protegin [®] XN	13344402	9
Caelo	Protegin [®] XN	13081907	3
Caelo	Protegin [®] XN	14220204	2
Caelo	Protegin [®] XN	14220203	2
Caelo	Protegin [®] XN	13344401	1
Caelo	Protegin [®] XN	14341301	3
Caelo	Protegin [®] XN	26031509	1
Caelo	Protegin [®] XN	14220208	3
Caelo	Protegin [®] XN	14220206	2
Caelo	Protegin [®] XN	14220208	1
Caelo	Protegin [®] XN	15252703	4
Caelo	Protegin [®] XN	15252702	2
Caelo	Protegin [®] XN	15252703	1
Caelo	Protegin [®] XN	16026703	3
Caelo	Protegin [®] XN	16026701	1
Caelo	Protegin [®] XN	16026707	7
Caelo	Protegin [®] XN	16026706	1
Caelo	Protegin [®] XN	16164502	2
Caelo	Protegin [®] XN	16164505	6
Caelo	Protegin [®] XN	16164507	1
Caelo	Protegin [®] XN	16164503	2
Caelo	Protegin [®] XN	17256702	1
Caelo	Protegin [®] XN	17258707	3
Caelo	Protegin [®] XN	20001749003	15
Caelo	Protegin [®] XN	200001749005	1
Caelo	Protegin [®] XN	20001749001	7
Caelo	Protegin [®] XN	2001749003	1
Caelo	Protegin [®] XN	13344402	2
Caelo	Protegin [®] XN	191092002/4820	1
Caelo	Protegin [®] XN	11196805	1
Caelo	Protegin [®] XN	20001749005	5
Caelo	Protegin [®] XN	22000510005	2
Caelo	Protegin [®] XN	16026704	5
Caelo	Protegin [®] XN	18059512	7
Caelo	Protegin [®] XN	13081902	3
Caelo	Protegin [®] XN	14220209	4
Caelo	Protegin [®] XN	16026702	6
Caelo	Protegin [®] XN	13081906	5
Caelo	Protegin [®] XN	14220203	1
Caelo	Protegin [®] XN	14220204	1
Caelo	Protegin [®] XN	16026709	3
Caelo	Protegin [®] XN	16164501	1
Caelo	Protegin [®] XN	16164504	1
Caelo	Protegin [®] XN	13081906	1
Caelo	Protegin [®] XN	14341302	1
Caelo	Protegin [®] XN	11196801	1
Caelo	Protegin [®] XN	13344401	5
Caelo	Protegin [®] XN	17258702	1
Caelo	Protegin [®] XN	21003187003	12
Caelo	Protegin [®] XN	21003187006	5
Caelo	Protegin [®] XN	17258705	1
Caelo	Protegin [®] XN	1910920002	1
Caelo	Protegin [®] XN	17258708	2
Caelo	Protegin [®] XN	20001749007	13
Caelo	Protegin [®] XN	14220202	5

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Supplier	Substance	Batch	Spectra
Caelo	Protegin [®] XN	16026701	7
Caelo	Protegin [®] XN	1805907	1
Caelo	Protegin [®] XN	18059505	2
Caelo	Protegin [®] XN	18059509	1
Caelo	Protegin [®] XN	20001749012	4
Caelo	Protegin [®] XN	2000149012	1
Caelo	Protegin [®] XN	22000510002	8
Caelo	Protegin [®] XN	18059502	12
Caelo	Protegin [®] XN	18059503	2
Caelo	Protegin [®] XN	19109003	3
Caelo	Protegin [®] XN	19110202	35
Caelo	Protegin [®] XN	20001749013	3
Caelo	Protegin [®] XN	22000510004	7
Caelo	Protegin [®] XN	13081905	11
Caelo	Protegin [®] XN	14220201	1
Caelo	Protegin [®] XN	1805901	1
Caelo	Protegin [®] XN	19110201	13
Caelo	Protegin [®] XN	191092002	7
Caelo	Protegin [®] XN	21003187005	1
Caesar & Loretz	Protegin [®] XN	19109001	8
Caesar & Loretz GmbH	Protegin [®] XN	16164506	3
Caesar & Loretz GmbH	Protegin [®] XN	18059511	3
Caesar & Loretz GmbH	Protegin [®] XN	19109002	37
Caesar & Loretz GmbH	Protegin [®] XN	191092001	1
Caesar & Loretz GmbH	Protegin [®] XN	22000510009	1
Caesar & Loretz Gm...	Protegin [®] XN	21003187001	12
Caesar & Loretz Gm...	Protegin [®] XN	20001749009	2
Euro OTC	Protegin [®] XN	Ch.B250118B	1
GEHE	Protegin [®] XN	18059507	11
Hedinger/Phönix	Protegin [®] XN	18059501	17
Ichthyol-Gesellschaft	Protegin [®] XN	17258703	4
Kehr	Protegin [®] XN	1805607	1
Caelo	Protegin [®] XN	20001749010	10
Max Jenne	Protegin [®] XN	23002995008	4
Noweda	Protegin [®] XN	21003187002	1
Phoenix	Protegin [®] XN	22000510007	4
phönix	Protegin [®] XN	23002995006	1
Phönix	Protegin [®] XN	11196706	1
Phönix	Protegin [®] XN	13081901	7
Phönix	Protegin [®] XN	20001749004	4
Phönix 12.03.2013	Protegin [®] XN	12229205	1
Caelo	Protegin [®] XN	191090001	2
Caelo	Protegin [®] XN	14220205	6

R

Supplier	Substance	Batch	Spectra
Dyckerhoff	Regeneresen	60611dü-2	1
Dyckerhoff	Regeneresen	150173th-2	1
Dyckerhoff	Regeneresen	1202920v-2	1
Dyckerhoff	Regeneresen	120323Lu-2	1
Dyckerhoff	Regeneresen	120313Kn-2	1
Dyckerhoff	Regeneresen	1503839-Na	1
Dyckerhoff	Regeneresen	120333NN-2	1
Dyckerhoff	Regeneresen	120053NNR-2	1
Retterspitz/ Phoenix	Retterspitz external	17224	1
Retterspitz/ Phoenix	Retterspitz external	18045	1
Arkeo Immun UG	Rizol raw material	1192HJ	2

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Supplier	Substance	Batch	Spectra
Caelo	Rizol raw material	15144304	1
Steidl/Phytolab	Rizol raw material	200812174102290	1

S

Supplier	Substance	Batch	Spectra
Bombastus	Salicylic white paraffin 10%	298081	1
Bombastus	Salicylic white paraffin 10%	19004850	1
Bombastus	Salicylic white paraffin 10%	19003777	1
Bombastus	Salicylic white paraffin 10%	17000464	1
Bombastus	Salicylic white paraffin 10%	293212	1
Caelo	Salicylic white paraffin 10%	16120701	2
Caelo	Salicylic white paraffin 10%	15394702	1
Caelo	Salicylic white paraffin 10%	19058602	1
Caelo	Salicylic white paraffin 10%	19140602	1
Caelo	Salicylic white paraffin 10%	16214203	1
Caelo	Salicylic white paraffin 10%	16214202	1
Caelo	Salicylic white paraffin 10%	18245603	1
Caelo	Salicylic white paraffin 10%	18114703	1
Caelo	Salicylic white paraffin 10%	19140601	2
Caelo	Salicylic white paraffin 10%	29119140602	1
Eigenrezeptur	Salicylic white paraffin 10%	150702	1
hecht	Salicylic white paraffin 10%	80117.64	1
Hecht Pharma GmbH	Salicylic white paraffin 10%	80048-20	1
...			
Medicon Apotheke D...	Salicylic white paraffin 10%	4818J-07017	1
Caelo	Salicylic white paraffin 10%	21000468001	1
Winthrop	Salicylic white paraffin 10%	GA0926	1
Zentiva Pharma GmbH	Salicylic white paraffin 10%	IE6931	2
Sanacorp	Salmon oil	20003591001	1
	Sebexol® basic pH 5 formula...	2316117	15
	Sebexol® basic pH 5 formula...	2316117/	1
	Sebexol® basic pH 5 formula...	2427103	7
AHD	Sebexol® basic pH 5 formula...	1552.2	1
Bombastus	Sebexol® basic pH 5 formula...	1346	3
Caelo	Sebexol® basic pH 5 formula...	1239	2
Caelo	Sebexol® basic pH 5 formula...	1131	2
devesa	Sebexol® basic pH 5 formula...	2149108	10
Devesa	Sebexol® basic pH 5 formula...	I307	1
Devesa	Sebexol® basic pH 5 formula...	I232	1
Devesa	Sebexol® basic pH 5 formula...	1307	6
Devesa	Sebexol® basic pH 5 formula...	1210/03.2015	1
Devesa	Sebexol® basic pH 5 formula...	1103/01.2014	1
Devesa	Sebexol® basic pH 5 formula...	1307/02.2016	1
Devesa	Sebexol® basic pH 5 formula...	1328	17
Devesa	Sebexol® basic pH 5 formula...	1335	2
Devesa	Sebexol® basic pH 5 formula...	1404	1
Devesa	Sebexol® basic pH 5 formula...	1511	5
Devesa	Sebexol® basic pH 5 formula...	1522	4
Devesa	Sebexol® basic pH 5 formula...	1604127	10
Devesa	Sebexol® basic pH 5 formula...	1683124	1
Devesa	Sebexol® basic pH 5 formula...	1828110	12
Devesa	Sebexol® basic pH 5 formula...	1912118	8
Devesa	Sebexol® basic pH 5 formula...	1923107	16
Devesa	Sebexol® basic pH 5 formula...	1912118/03.2022	1
Devesa	Sebexol® basic pH 5 formula...	2009126/02	1
Devesa	Sebexol® basic pH 5 formula...	2031128	34
Devesa	Sebexol® basic pH 5 formula...	2102114	23
Devesa	Sebexol® basic pH 5 formula...	214910812	1

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Supplier	Substance	Batch	Spectra
DEVESA	Sebexol [®] basic pH 5 formula...	1318	2
DEVESA	Sebexol [®] basic pH 5 formula...	1807113	9
DEVESA	Sebexol [®] basic pH 5 formula...	185119	1
Devesa / Noweda	Sebexol [®] basic pH 5 formula...	170420S/1620117	1
Devesa / Noweda	Sebexol [®] basic pH 5 formula...	170516S/1644102	1
Devesa Dr.Reingrab...	Sebexol [®] basic pH 5 formula...	1425	4
Devesa Dr.Reingrab...	Sebexol [®] basic pH 5 formula...	2045106	1
Devesa Dr.Reingrab...	Sebexol [®] basic pH 5 formula...	1244	1
Devesa/ Fiebig	Sebexol [®] basic pH 5 formula...	1338	1
Devesa/ Phoenix	Sebexol [®] basic pH 5 formula...	2127106	5
Devesa/AHD	Sebexol [®] basic pH 5 formula...	1245	4
Devesa/alliance	Sebexol [®] basic pH 5 formula...	2316117/04	1
Devesa/Alliance	Sebexol [®] basic pH 5 formula...	2009126	24
devesa/gehe	Sebexol [®] basic pH 5 formula...	1356	1
Devesa/Gehe	Sebexol [®] basic pH 5 formula...	1313/03.2016	1
Devesa/Gehe	Sebexol [®] basic pH 5 formula...	1935126	17
Devesa/Gehe	Sebexol [®] basic pH 5 formula...	1946114	14
Devesa/Kehr	Sebexol [®] basic pH 5 formula...	1946114/11	1
Devesa/Noweda	Sebexol [®] basic pH 5 formula...	1430	3
Devesa/Noweda	Sebexol [®] basic pH 5 formula...	1719111/05	1
Devesa/Noweda	Sebexol [®] basic pH 5 formula...	1828110/07	1
Devesa/Phoenix	Sebexol [®] basic pH 5 formula...	2124115	27
Devesa/Phoenix	Sebexol [®] basic pH 5 formula...	2304125	3
DEVESA/Phoenix	Sebexol [®] basic pH 5 formula...	1446/11	1
Devesa/Phönix	Sebexol [®] basic pH 5 formula...	1712122	13
Devesa/Sanacorp	Sebexol [®] basic pH 5 formula...	1543	14
Devesa/Sanacorp	Sebexol [®] basic pH 5 formula...	1620117	10
Devesa/Sanacorp	Sebexol [®] basic pH 5 formula...	1638124	9
Devesa/Sanacorp	Sebexol [®] basic pH 5 formula...	1719111	12
Devesa/Sanacorp	Sebexol [®] basic pH 5 formula...	1817126	11
Devesa/Sanacorp	Sebexol [®] basic pH 5 formula...	187126/06	1
Devesa/Sanacorp	Sebexol [®] basic pH 5 formula...	1851119	11
Devesa/Sanacorp	Sebexol [®] basic pH 5 formula...	2243126	3
Dr. Reingraber GmbH	Sebexol [®] basic pH 5 formula...	1708120	1
Dr.Reingraber GmbH	Sebexol [®] basic pH 5 formula...	1232	4
Fagron	Sebexol [®] basic pH 5 formula...	1510	2
kehr	Sebexol [®] basic pH 5 formula...	2436104	4
Kehr/ Devesa	Sebexol [®] basic pH 5 formula...	1644102	15
Kehr/ Devesa	Sebexol [®] basic pH 5 formula...	1746116	8
Noweda/Devesa	Sebexol [®] basic pH 5 formula...	2x1407	1
Phoenix	Sebexol [®] basic pH 5 formula...	1440	11
Phoenix/Devesa	Sebexol [®] basic pH 5 formula...	1215	1
Phoenix/Devesa	Sebexol [®] basic pH 5 formula...	1407	5
Phönix	Sebexol [®] basic pH 5 formula...	1313	4
Phönix	Sebexol [®] basic pH 5 formula...	1416	1
Sanacorp	Sebexol [®] basic pH 5 formula...	2337114	1
Sebexol	Sebexol [®] basic pH 5 formula...	1333	1
Sebexol/ Noweda	Sebexol [®] basic pH 5 formula...	1403	1
Sebexol/AHD	Sebexol [®] basic pH 5 formula...	1303	3
	Sebexol [®] cream lotion	2304125	11
	Sebexol [®] cream lotion	2304126	16
	Sebexol [®] cream lotion	2316119	18
	Sebexol [®] cream lotion	2338120	16
	Sebexol [®] cream lotion	2414103	26
	Sebexol [®] cream lotion		3
	Sebexol [®] cream lotion	2414402	1

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Supplier	Substance	Batch	Spectra
	Sebexol [®] cream lotion	241410	1
	Sebexol [®] cream lotion	2427103	14
	Sebexol [®] cream lotion	2436109	1
	Sebexol [®] cream lotion	2436105	8
	Sebexol [®] cream lotion	2436106	13
	Sebexol [®] cream lotion	2513224	1
Astellas	Sebexol [®] cream lotion	1504	8
Caelo	Sebexol [®] cream lotion	1552.4	1
Caelo	Sebexol [®] cream lotion	1417	1
Caelo	Sebexol [®] cream lotion	4117E-03872	1
Caelo	Sebexol [®] cream lotion	1605101	6
Caelo	Sebexol [®] cream lotion	1836106	7
Caelo	Sebexol [®] cream lotion	19031605	1
Caelo	Sebexol [®] cream lotion	1531	3
Caelo	Sebexol [®] cream lotion	1552.3	3
Caelo	Sebexol [®] cream lotion	1912119	14
deversa	Sebexol [®] cream lotion	1935227	27
Deves/Phönix	Sebexol [®] cream lotion	2127109	8
Devesa	Sebexol [®] cream lotion	1510	5
Devesa	Sebexol [®] cream lotion	1524	3
Devesa	Sebexol [®] cream lotion	1552.2	2
Devesa	Sebexol [®] cream lotion	1522.2	1
Devesa	Sebexol [®] cream lotion	1604128	2
Devesa	Sebexol [®] cream lotion	1651121	8
Devesa	Sebexol [®] cream lotion	1708120	11
Devesa	Sebexol [®] cream lotion	1417N-03872	1
Devesa	Sebexol [®] cream lotion	1746116	20
Devesa	Sebexol [®] cream lotion	1817127	9
Devesa	Sebexol [®] cream lotion	181223/	1
Devesa	Sebexol [®] cream lotion	1923108	24
Devesa	Sebexol [®] cream lotion	1925120	1
Devesa	Sebexol [®] cream lotion	1923108/06.2022	1
Devesa	Sebexol [®] cream lotion	1923108/06-2022	1
Devesa	Sebexol [®] cream lotion	7/02.202003	1
Devesa	Sebexol [®] cream lotion	201907	1
Devesa	Sebexol [®] cream lotion	2103120	16
Devesa	Sebexol [®] cream lotion	9072021	1
Devesa	Sebexol [®] cream lotion	2124116	17
Devesa	Sebexol [®] cream lotion	2124117	15
Devesa	Sebexol [®] cream lotion	212701	1
Devesa	Sebexol [®] cream lotion	250322/1	1
DEVESA	Sebexol [®] cream lotion	1505	1
DEVESA	Sebexol [®] cream lotion	1523	6
DEVESA	Sebexol [®] cream lotion	1651120	5
DEVESA	Sebexol [®] cream lotion	1802108/01	2
DEVESA	Sebexol [®] cream lotion	2243128	11
Devesa /	Sebexol [®] cream lotion	1511	6
Devesa /	Sebexol [®] cream lotion	1812223	14
Devesa / Gehe	Sebexol [®] cream lotion	1517	2
Devesa / Gehe	Sebexol [®] cream lotion	1543,20160225/3	1
Devesa / Gehe	Sebexol [®] cream lotion	2009127	15
Devesa / Gehe	Sebexol [®] cream lotion	2009126	1
Devesa / Gehe 08.12.18	Sebexol [®] cream lotion	1824215-S20190115Ma7	1
Devesa / Gehe 15.3.18	Sebexol [®] cream lotion	1743225-20180404Ma10	1
Devesa / Noweda	Sebexol [®] cream lotion	1430	2
Devesa /Gehe	Sebexol [®] cream lotion	1901103	22

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Supplier	Substance	Batch	Spectra
Devesa /Phönix	Sebexol [®] cream lotion	1807113	19
DEVESA Dr. Rein- gra...	Sebexol [®] cream lotion	2149108	6
DEVESA Dr. Rein- gra...	Sebexol [®] cream lotion	21281147	1
Devesa Dr.Reingrab...	Sebexol [®] cream lotion	174611650ml	1
Devesa Dr.Reingrab...	Sebexol [®] cream lotion	1935127	17
DEVESA Dr.Reingrab...	Sebexol [®] cream lotion	2128112	16
DEVESA Dr.Reingrab...	Sebexol [®] cream lotion	4/07.202004	1
devesa phoenix	Sebexol [®] cream lotion	1925121	20
Devesa-Fa.Gehe	Sebexol [®] cream lotion	1727207/-20180112Ma9	1
Devesa-Fa.Gehe	Sebexol [®] cream lotion	1824215-S20181115Ma2	1
Devesa/	Sebexol [®] cream lotion	1504-10,03,2015	1
Devesa/	Sebexol [®] cream lotion	1504-04,11,2015	1
Devesa/	Sebexol [®] cream lotion	17433225	1
Devesa/ Noweda	Sebexol [®] cream lotion	1736105	15
Devesa/ Noweda	Sebexol [®] cream lotion	1939227	19
Devesa/ Phoenix	Sebexol [®] cream lotion	1620117	1
DEVESA/ Phoenix	Sebexol [®] cream lotion	1939127/09	1
Devesa/ Phönix	Sebexol [®] cream lotion	1743225	5
Devesa/ Sanacorp	Sebexol [®] cream lotion	20042120	1
Devesa/AHD	Sebexol [®] cream lotion	2128114	18
Devesa/Alliance	Sebexol [®] cream lotion	2019207	15
Devesa/Anzag	Sebexol [®] cream lotion	2019107/05.2023	2
Devesa/Anzag	Sebexol [®] cream lotion	2128112/07.2024	1
Devesa/Fiebig	Sebexol [®] cream lotion	1426	1
Devesa/Fiebig	Sebexol [®] cream lotion	1947118.11	2
Devesa/Fiebig	Sebexol [®] cream lotion	1947118	30
Devesa/Fiebig	Sebexol [®] cream lotion	201107	2
Devesa/Fiebig	Sebexol [®] cream lotion	2045106	20
Devesa/Fiebig	Sebexol [®] cream lotion	2103119	19
Devesa/Fiebig	Sebexol [®] cream lotion	218112	2
Devesa/Gehe	Sebexol [®] cream lotion	1817227	15
Devesa/Gehe	Sebexol [®] cream lotion	2127108	24
Devesa/Gehe	Sebexol [®] cream lotion	6/01.202006	1
Devesa/Noveda	Sebexol [®] cream lotion	2124166	1
Devesa/NOW	Sebexol [®] cream lotion	1504/01	1
Devesa/NOW	Sebexol [®] cream lotion	1552	1
Devesa/NOW	Sebexol [®] cream lotion	1644102	7
Devesa/Noweda	Sebexol [®] cream lotion	1447	4
Devesa/Noweda	Sebexol [®] cream lotion	1552.1	3
Devesa/Noweda	Sebexol [®] cream lotion	1604228	7
Devesa/Noweda	Sebexol [®] cream lotion	1543	2
Devesa/Noweda	Sebexol [®] cream lotion	1719112	2
Devesa/Noweda	Sebexol [®] cream lotion	1736106	13
Devesa/Noweda	Sebexol [®] cream lotion	1901102	15
Devesa/Noweda	Sebexol [®] cream lotion	200412D	1
Devesa/Noweda	Sebexol [®] cream lotion	1947119/11	1
Devesa/Phoenix	Sebexol [®] cream lotion	2004120	30
DEVESA/PHOENIX	Sebexol [®] cream lotion	2019107	20
Devesa/Phömix	Sebexol [®] cream lotion	1712223	10
devesa/Phönix	Sebexol [®] cream lotion	1802208	13
devesa/Phönix	Sebexol [®] cream lotion	18201402	1
Devesa/Phönix	Sebexol [®] cream lotion	1824215	9
Devesa/Phönix	Sebexol [®] cream lotion	1828111	37

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Supplier	Substance	Batch	Spectra
Devesa/Phönix	Sebexol [®] cream lotion	1912120	20
Devesa/Phönix	Sebexol [®] cream lotion	1939127	17
Devesa/Phönix	Sebexol [®] cream lotion	1807113/02	1
Devesa/Phönix	Sebexol [®] cream lotion	2009227	32
Devesa/Phönix	Sebexol [®] cream lotion	19107	1
DEVESA/Phönix	Sebexol [®] cream lotion	185119	1
Devesa/Sanacorp	Sebexol [®] cream lotion	1743125	9
Devesa/Sanacorp	Sebexol [®] cream lotion	2040130	21
Euro OTC	Sebexol [®] cream lotion	1727207	4
Fa. Devesa/Noweda	Sebexol [®] cream lotion	1947119	30
Fa. Devesa/Noweda	Sebexol [®] cream lotion	2127208	23
Fiebig/Devesa	Sebexol [®] cream lotion	1836105	14
Gehe	Sebexol [®] cream lotion	1605103	4
Gehe	Sebexol [®] cream lotion	1727107	6
Gehe	Sebexol [®] cream lotion	2414102	9
Gehe	Sebexol [®] cream lotion	2513124	7
Hedinger/Noweda	Sebexol [®] cream lotion	18424115	1
infectopharm/Alliance	Sebexol [®] cream lotion	1817227/04	1
Noweda	Sebexol [®] cream lotion	1802108	4
Noweda	Sebexol [®] cream lotion	2046109	12
Noweda	Sebexol [®] cream lotion	2316118	16
Noweda	Sebexol [®] cream lotion	2316119/2311140	1
NOWEDA / HER- STELLE...	Sebexol [®] cream lotion	19471118, 11	1
Noweda/Devesa	Sebexol [®] cream lotion	1530	5
Noweda/Devesa	Sebexol [®] cream lotion	1605201	6
Noweda/Devesa	Sebexol [®] cream lotion	1720115	3
Noweda/Devesa	Sebexol [®] cream lotion	1638124	1
Phoenix/Devesa	Sebexol [®] cream lotion	1812123	10
Phönix	Sebexol [®] cream lotion	160422	1
Phönix	Sebexol [®] cream lotion	1604129	9
Phönix	Sebexol [®] cream lotion	4217A-03872	1
Phönix	Sebexol [®] cream lotion	2149110	20
Phönix/Devesa	Sebexol [®] cream lotion	1712123	5
Phönix/Devesa	Sebexol [®] cream lotion	1824115	15
Phönix/Devesa	Sebexol [®] cream lotion	182811	1
Sanacorp	Sebexol [®] cream lotion	2337114	17
sanacorp, 27.9.16,...	Sebexol [®] cream lotion	1604328	7
Taosis	Sebexol [®] cream lotion	1828110	6
	Solutio Cordes [®]	22B0003	6
	Solutio Cordes [®]	21B0003	1
cordes hermann & co	Solutio Cordes [®]	16B010	2
Cordes/Sanacorp	Solutio Cordes [®]	19B005	3
Fiebig	Solutio Cordes [®]	22314	1
Gehe/Ichthyol	Solutio Cordes [®]	14b006	1
Ichthol/ Noweda 13...	Solutio Cordes [®]	17b007	1
ichthyol	Solutio Cordes [®]	14B012	1
ichthyol	Solutio Cordes [®]	17B008	2
Ichthyol	Solutio Cordes [®]	13B001	2
Ichthyol	Solutio Cordes [®]	14B012	4
Ichthyol	Solutio Cordes [®]	15B005	5
Ichthyol	Solutio Cordes [®]	198004	1
Ichthyol	Solutio Cordes [®]	19007	1
Ichthyol / G	Solutio Cordes [®]	16B005	3
Ichthyol / Gehe	Solutio Cordes [®]	14B006	2
Ichthyol /Noweda	Solutio Cordes [®]	138002	1

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Supplier	Substance	Batch	Spectra
Ichthyol- Gesellsc. . .	Solutio Cordes [®]	13B001	1
Ichthyol-Gesellsch. . .	Solutio Cordes [®]	188004	1
Ichthyol-Gesellsch. . .	Solutio Cordes [®]	20B0008	4
Ichthyol/AHCA	Solutio Cordes [®]	17B007	10
Ichthyol/Phönix	Solutio Cordes [®]	12B0005	1
Ichthyol/Phönix	Solutio Cordes [®]	12B005	17
Ichthyol/Phönix	Solutio Cordes [®]	13B002	5
Ichthyol/Phönix	Solutio Cordes [®]	14B011	5
Ichthyol/Phönix	Solutio Cordes [®]	15B001	3
Ichthyol/Sanacorp	Solutio Cordes [®]	19B007	1
Ichtyol	Solutio Cordes [®]	12B006	3
Ichtyol / Gehe	Solutio Cordes [®]	2080008	1
Ichtyol-Gesellscha. . .	Solutio Cordes [®]	200008	1
Noweda	Solutio Cordes [®]	18B004	12
Phoenix	Solutio Cordes [®]	24B0001	1
apomix	Stomahesive [®] adhesive paste	9B033	2
ConvaTec/ Alliance	Stomahesive [®] adhesive paste	9K007	2
ConvaTec/Anzag	Stomahesive [®] adhesive paste	5G062	25
Convatec/Gehe	Stomahesive [®] adhesive paste	9D046	1
Convatec/Phönix	Stomahesive [®] adhesive paste	6D079	1
	SyrSpend [®] SF pH4 cherry aroma	23A10-T20-102143	7
	SyrSpend [®] SF pH4 cherry aroma	23a26-to3-102457	1
	SyrSpend [®] SF pH4 cherry aroma	2103078	1
	SyrSpend [®] SF pH4 cherry aroma	23A10-T20	2
	SyrSpend [®] SF pH4 cherry aroma	22H11-T09-099022	1
	SyrSpend [®] SF pH4 cherry aroma	23B17-T02-103078	8
	SyrSpend [®] SF pH4 cherry aroma	23A10-T20-102144	1
	SyrSpend [®] SF pH4 cherry aroma	23c08-t04-103682	1
	SyrSpend [®] SF pH4 cherry aroma	22I14-T22-099449	6
	SyrSpend [®] SF pH4 cherry aroma	23D05-T03-104272	7
	SyrSpend [®] SF pH4 cherry aroma	22J14-T08-1000064	1
	SyrSpend [®] SF pH4 cherry aroma	23C08-T03-103676	23
	SyrSpend [®] SF pH4 cherry aroma	22C13-T06-103720	1
	SyrSpend [®] SF pH4 cherry aroma	23C08-T03	5
	SyrSpend [®] SF pH4 cherry aroma	23B17-T02	2
	SyrSpend [®] SF pH4 cherry aroma	23A26-T03	2
	SyrSpend [®] SF pH4 cherry aroma	T0510246000	1
	SyrSpend [®] SF pH4 cherry aroma	23A26-T05-102460	3
	SyrSpend [®] SF pH4 cherry aroma	23C08-T04-103682	5
	SyrSpend [®] SF pH4 cherry aroma	23C13-T06-103720	12
	SyrSpend [®] SF pH4 cherry aroma	23D05-T04-104277	4
	SyrSpend [®] SF pH4 cherry aroma	fagron	1
	SyrSpend [®] SF pH4 cherry aroma	22H11T13099034	1
	SyrSpend [®] SF pH4 cherry aroma	23C08-T04	3
	SyrSpend [®] SF pH4 cherry aroma	23D05-T05-099074	2
	SyrSpend [®] SF pH4 cherry aroma	23C08-T03-103676	1
	SyrSpend [®] SF pH4 cherry aroma	23C08-T03-1036709	1
	SyrSpend [®] SF pH4 cherry aroma	23C13-T06	1
	SyrSpend [®] SF pH4 cherry aroma	22/14-T22-099449	1
	SyrSpend [®] SF pH4 cherry aroma	23C13-T07-103723	10
	SyrSpend [®] SF pH4 cherry aroma	T13_0990304	1
	SyrSpend [®] SF pH4 cherry aroma	23C13-T07	3
	SyrSpend [®] SF pH4 cherry aroma	23817-T02-103078	1
	SyrSpend [®] SF pH4 cherry aroma	T07-1037203	7
	SyrSpend [®] SF pH4 cherry aroma	23C13-T07-1037203	1
	SyrSpend [®] SF pH4 cherry aroma	23E22-T14-1054407	1

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Supplier	Substance	Batch	Spectra
	SyrSpend [®] SF pH4 cherry aroma	22HT11-T13-099034	1
	SyrSpend [®] SF pH4 cherry aroma	23E22-T14-105447	3
	SyrSpend [®] SF pH4 cherry aroma	23E22-T14	3
	SyrSpend [®] SF pH4 cherry aroma	2398472893465	1
	SyrSpend [®] SF pH4 cherry aroma	23E12-T02-105247	12
	SyrSpend [®] SF pH4 cherry aroma	23F14-T12-106215	11
	SyrSpend [®] SF pH4 cherry aroma	T02-1052407	6
	SyrSpend [®] SF pH4 cherry aroma	23E22-T15-1054505	1
	SyrSpend [®] SF pH4 cherry aroma	T05-1054107	4
	SyrSpend [®] SF pH4 cherry aroma	22H11-T11	1
	SyrSpend [®] SF pH4 cherry aroma	23E12-T02	2
	SyrSpend [®] SF pH4 cherry aroma	23E12-T02-1052407	4
	SyrSpend [®] SF pH4 cherry aroma	23c08-t03-103676	1
	SyrSpend [®] SF pH4 cherry aroma	23D05T03104272	1
	SyrSpend [®] SF pH4 cherry aroma	To7_1037203	1
	SyrSpend [®] SF pH4 cherry aroma	T14-1054407	1
	SyrSpend [®] SF pH4 cherry aroma	23F14-T12	1
	SyrSpend [®] SF pH4 cherry aroma	23E12-T02	1
	SyrSpend [®] SF pH4 cherry aroma	23E22-T05	2
	SyrSpend [®] SF pH4 cherry aroma	T01-1030708	1
	SyrSpend [®] SF pH4 cherry aroma	23E-T05-105417	1
	SyrSpend [®] SF pH4 cherry aroma	23E22-T06-105420	1
	SyrSpend [®] SF pH4 cherry aroma	23C13T06103720	1
	SyrSpend [®] SF pH4 cherry aroma	25G17-T05-123204	1
	SyrSpend [®] SF pH4 cherry aroma	25G17-T05-123203	1
	SyrSpend [®] SF pH4 cherry aroma	25G25-T06-124284	1
Alliance	SyrSpend [®] SF pH4 cherry aroma	23E22-T05-105417	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	20006936	21
Anzag	SyrSpend [®] SF pH4 cherry aroma	231213(23A26-T03-102457)1	
Anzag	SyrSpend [®] SF pH4 cherry aroma	240115(23A26-T03-102457)1	
Anzag	SyrSpend [®] SF pH4 cherry aroma	240228(23A26-T03-102457)1	
Anzag	SyrSpend [®] SF pH4 cherry aroma	240412(23A26-T03-102457)1	
Anzag	SyrSpend [®] SF pH4 cherry aroma	240507(23A26-T03-102457)1	
Anzag	SyrSpend [®] SF pH4 cherry aroma	240530(23A26-T03-102457)1	
Anzag	SyrSpend [®] SF pH4 cherry aroma	240726(23A26-T03-102457)1	
Anzag	SyrSpend [®] SF pH4 cherry aroma	241212	1
Anzag	SyrSpend [®] SF pH4 cherry aroma	23E22-T05-105417	24
Anzag	SyrSpend [®] SF pH4 cherry aroma	250220(23E22-T05-105417)1	
Anzag	SyrSpend [®] SF pH4 cherry aroma	250428(23E22-T05-105417)1	
Anzag	SyrSpend [®] SF pH4 cherry aroma	250512(23E22-T05-105417)1	
Caelo	SyrSpend [®] SF pH4 cherry aroma	1900093P-190927-2	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1806233/2P-190927-3	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1800673/1	25
Caelo	SyrSpend [®] SF pH4 cherry aroma	1806233/02	1
Caelo	SyrSpend [®] SF pH4 cherry aroma	1612631,	1
Caesar & Loretz GmbH	SyrSpend [®] SF pH4 cherry aroma	19000779004	1
Caesar & Loretz GmbH	SyrSpend [®] SF pH4 cherry aroma	21000431001	1
Caesar & Loretz GmbH	SyrSpend [®] SF pH4 cherry aroma	21001852006	1
Euro OTC	SyrSpend [®] SF pH4 cherry aroma	1704492/01	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	200000326	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	1503D017	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	15C19/C	9
Fagron	SyrSpend [®] SF pH4 cherry aroma	1507318	8
Fagron	SyrSpend [®] SF pH4 cherry aroma	1503255	20
Fagron	SyrSpend [®] SF pH4 cherry aroma	1603252/2	13
Fagron	SyrSpend [®] SF pH4 cherry aroma	1612631	23

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Supplier	Substance	Batch	Spectra
Fagron	SyrSpend [®] SF pH4 cherry aroma	1701543/3	5
Fagron	SyrSpend [®] SF pH4 cherry aroma	1707302/1	9
Fagron	SyrSpend [®] SF pH4 cherry aroma	1702015(2Flaschen)	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	2x1712024	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1800673/2	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1806233/2	41
Fagron	SyrSpend [®] SF pH4 cherry aroma	1806233/2P-190618-2	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	19009673	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	2000326	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	20004221	17
Fagron	SyrSpend [®] SF pH4 cherry aroma	2006936	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	20004369	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	200007312	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	21002532	74
Fagron	SyrSpend [®] SF pH4 cherry aroma	21020483	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	21008809	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	22B24-T01	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	T18-0959108	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11-T18-095918	10
Fagron	SyrSpend [®] SF pH4 cherry aroma	T17-0959100	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11-T18-05918	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11-T17-095911	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T13-099035	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	22J14-T08-100065	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H30-T05-099074	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T17-095910	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T13	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	22J14-T08	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22J14-T08	5
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-TT18-099038	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H13-099035	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	23A26-T03	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	T13-0990305	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	23A05-T07-102866	9
Fagron	SyrSpend [®] SF pH4 cherry aroma	21010483	59
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T11-099029	8
Fagron	SyrSpend [®] SF pH4 cherry aroma	1802928	6
Fagron	SyrSpend [®] SF pH4 cherry aroma	22J14-T08-100065	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	1909673	69
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11-T17-095910	23
Fagron	SyrSpend [®] SF pH4 cherry aroma	720023-0003	5
Fagron	SyrSpend [®] SF pH4 cherry aroma	1908041	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T18-099038	33
Fagron	SyrSpend [®] SF pH4 cherry aroma	22I14-T22	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	A05-T07-1028606	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	23A05-T07-102866	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	23A26-T03-102457	26
Fagron	SyrSpend [®] SF pH4 cherry aroma	T20-1021403	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1806233/1	5
Fagron	SyrSpend [®] SF pH4 cherry aroma	20007317	23
Fagron	SyrSpend [®] SF pH4 cherry aroma	1800673/1P-180827-1	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1803724/2P-180922-1	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1806233/2P-190808-3	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	20000326P-200709-3	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	20007312,	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	518E-07041	1

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Supplier	Substance	Batch	Spectra
Fagron	SyrSpend [®] SF pH4 cherry aroma	200047312	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T11-099030	6
Fagron	SyrSpend [®] SF pH4 cherry aroma	1707032/1	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1712017	8
Fagron	SyrSpend [®] SF pH4 cherry aroma	1704492/1	11
Fagron	SyrSpend [®] SF pH4 cherry aroma	4415A-07041	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1860233/2	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1909423/1	22
Fagron	SyrSpend [®] SF pH4 cherry aroma	1904383	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1909423/2	5
Fagron	SyrSpend [®] SF pH4 cherry aroma	1909423-2	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	20007125	58
Fagron	SyrSpend [®] SF pH4 cherry aroma	T17-095910	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1712024	23
Fagron	SyrSpend [®] SF pH4 cherry aroma	20004332	64
Fagron	SyrSpend [®] SF pH4 cherry aroma	18062331	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	190973	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1800673	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11T17095910	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22J14-T08-100064	12
Fagron	SyrSpend [®] SF pH4 cherry aroma	20007312	77
Fagron	SyrSpend [®] SF pH4 cherry aroma	18000673/1	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1704992/1	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	1702015	33
Fagron	SyrSpend [®] SF pH4 cherry aroma	1911010	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	20007312mfa	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	20007130	12
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T13-099034	13
Fagron	SyrSpend [®] SF pH4 cherry aroma	22H11-T18	4
Fagron	SyrSpend [®] SF pH4 cherry aroma	22j14-t08-100064	3
Fagron	SyrSpend [®] SF pH4 cherry aroma	21005761	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	2007312	2
Fagron	SyrSpend [®] SF pH4 cherry aroma	1900093	34
Fagron	SyrSpend [®] SF pH4 cherry aroma	20000326	96
Fagron	SyrSpend [®] SF pH4 cherry aroma	13359004	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	180067/1	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	19094231	1
gehe	SyrSpend [®] SF pH4 cherry aroma	23a26-T05-102460	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	17122017	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	20007152	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	23A26-T03-102457	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	23C13_T07	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	23E22T05-105417	1
Gehe	SyrSpend [®] SF pH4 cherry aroma	23E22-T04-105414	1
GEHE	SyrSpend [®] SF pH4 cherry aroma	1803724/2	42
Caelo	SyrSpend [®] SF pH4 cherry aroma	1704492	1
kehr	SyrSpend [®] SF pH4 cherry aroma	22H11T11099029	1
Kehr	SyrSpend [®] SF pH4 cherry aroma	22114-T22-099449	2
noweda	SyrSpend [®] SF pH4 cherry aroma	22114-T22-099449	1
Noweda	SyrSpend [®] SF pH4 cherry aroma	22/14-T08-100064	2
Noweda	SyrSpend [®] SF pH4 cherry aroma	23E12-T02-105247	1
Phönix	SyrSpend [®] SF pH4 cherry aroma	21.01.25022	1
Phönix	SyrSpend [®] SF pH4 cherry aroma	22D11-T17	2
Phönix	SyrSpend [®] SF pH4 cherry aroma	23E22-T15-105455	1
Phönix	SyrSpend [®] SF pH4 cherry aroma	23E12-T02.105247	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	19094223/2	1

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Supplier	Substance	Batch	Spectra
Fagron	SyrSpend [®] SF pH4 cherry aroma	180623312	1
Fagron	SyrSpend [®] SF pH4 cherry aroma	22D11-T18	3
	SyrSpend [®] SF pH4 aroma free	23B10-T02	2
	SyrSpend [®] SF pH4 aroma free	23b10-t02-102920	2
	SyrSpend [®] SF pH4 aroma free	22h11-t09-099022	1
	SyrSpend [®] SF pH4 aroma free	23b17-t03-103125	1
	SyrSpend [®] SF pH4 aroma free	22h11-t09	1
	SyrSpend [®] SF pH4 aroma free	23B17T03103125	1
	SyrSpend [®] SF pH4 aroma free	23b09-T05-102908	1
	SyrSpend [®] SF pH4 aroma free	23B17-T03-103125	5
	SyrSpend [®] SF pH4 aroma free	22H11-T10-	1
	SyrSpend [®] SF pH4 aroma free	23817-T03-103124	1
	SyrSpend [®] SF pH4 aroma free	2200887	1
	SyrSpend [®] SF pH4 aroma free	23A16-T09-102195	9
	SyrSpend [®] SF pH4 aroma free	23B17-T03-103124	22
	SyrSpend [®] SF pH4 aroma free	23a24-T16-106100	1
	SyrSpend [®] SF pH4 aroma free	23A16-T09	1
	SyrSpend [®] SF pH4 aroma free	23B10-T03-102920	1
	SyrSpend [®] SF pH4 aroma free	116-106100	1
	SyrSpend [®] SF pH4 aroma free	23a24-t16-106100	1
	SyrSpend [®] SF pH4 aroma free	22J04-F02-383639	1
	SyrSpend [®] SF pH4 aroma free	23A24-T16-1061000	1
	SyrSpend [®] SF pH4 aroma free	23E19T17-105395	1
	SyrSpend [®] SF pH4 aroma free	23A24-T16	6
	SyrSpend [®] SF pH4 aroma free	23B02-T16-106340	7
	SyrSpend [®] SF pH4 aroma free	T16-1061000	8
	SyrSpend [®] SF pH4 aroma free	23E19-T17-105395	10
	SyrSpend [®] SF pH4 aroma free	23A16-T09-102194	3
	SyrSpend [®] SF pH4 aroma free	23BT17-T03-103125	1
	SyrSpend [®] SF pH4 aroma free	23B02-T16-106339	7
	SyrSpend [®] SF pH4 aroma free	9-09589008	1
	SyrSpend [®] SF pH4 aroma free	23A24-T16-1206100	1
	SyrSpend [®] SF pH4 aroma free	T17-1053905	6
	SyrSpend [®] SF pH4 aroma free	T16-106100	1
	SyrSpend [®] SF pH4 aroma free	23B09	1
	SyrSpend [®] SF pH4 aroma free	13359062	1
	SyrSpend [®] SF pH4 aroma free	23B09-T05	2
	SyrSpend [®] SF pH4 aroma free	T02-1029200	1
	SyrSpend [®] SF pH4 aroma free	23B17-T03	3
	SyrSpend [®] SF pH4 aroma free	T09-1035109	1
	SyrSpend [®] SF pH4 aroma free	23B02-T16-106340	1
	SyrSpend [®] SF pH4 aroma free	23B24-T09-103519	7
	SyrSpend [®] SF pH4 aroma free	22D11-09-095898	1
	SyrSpend [®] SF pH4 aroma free	T12-1053706	9
	SyrSpend [®] SF pH4 aroma free	23E19-T12-105376	12
	SyrSpend [®] SF pH4 aroma free	23E19-T-105395	1
	SyrSpend [®] SF pH4 aroma free	23E19-T17	1
	SyrSpend [®] SF pH4 aroma free	23B24-T09	1
	SyrSpend [®] SF pH4 aroma free	24G11-T03-115196	4
	SyrSpend [®] SF pH4 aroma free	23E19-T15-105387	15
	SyrSpend [®] SF pH4 aroma free	23E19-T12-1053706	1
	SyrSpend [®] SF pH4 aroma free	T15-1053807	8
	SyrSpend [®] SF pH4 aroma free	24G11-T03-115196	1
	SyrSpend [®] SF pH4 aroma free	T03-1151906	2
	SyrSpend [®] SF pH4 aroma free	T17-1053904	2
	SyrSpend [®] SF pH4 aroma free	24K20-T02-117948	11

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Supplier	Substance	Batch	Spectra
	SyrSpend [®] SF pH4 aroma free	23E19-T15-1053807	1
	SyrSpend [®] SF pH4 aroma free	23E19-T16	1
	SyrSpend [®] SF pH4 aroma free	23E19-T15	1
	SyrSpend [®] SF pH4 aroma free	23E19-T16-10053900	1
	SyrSpend [®] SF pH4 aroma free	23E19-T12-10576	1
	SyrSpend [®] SF pH4 aroma free	23F19-T16-105390	1
	SyrSpend [®] SF pH4 aroma free	25B07-T04-119651	3
	SyrSpend [®] SF pH4 aroma free	24K20-T02	1
	SyrSpend [®] SF pH4 aroma free	25B07-T04	1
	SyrSpend [®] SF pH4 aroma free	23e19-t15-105387	1
	SyrSpend [®] SF pH4 aroma free	23F16-T02-106346	1
	SyrSpend [®] SF pH4 aroma free	25H21-T02	1
AHD	SyrSpend [®] SF pH4 aroma free	22H1-T09-099022	1
Anzag	SyrSpend [®] SF pH4 aroma free	23B09-T05-102908	18
Anzag	SyrSpend [®] SF pH4 aroma free	23B02-T16	2
Caelo	SyrSpend [®] SF pH4 aroma free	19061126	1
Caelo	SyrSpend [®] SF pH4 aroma free	1812018	1
Fagron	SyrSpend [®] SF pH4 aroma free	22D11T09095898	1
Fagron	SyrSpend [®] SF pH4 aroma free	23B09-t05	1
Fagron	SyrSpend [®] SF pH4 aroma free	1410D020	9
Fagron	SyrSpend [®] SF pH4 aroma free	15C12/E	1
Fagron	SyrSpend [®] SF pH4 aroma free	15C12E	1
Fagron	SyrSpend [®] SF pH4 aroma free	1609686	1
Fagron	SyrSpend [®] SF pH4 aroma free	1706769/1	7
Fagron	SyrSpend [®] SF pH4 aroma free	1706769	1
Fagron	SyrSpend [®] SF pH4 aroma free	1712018	9
Fagron	SyrSpend [®] SF pH4 aroma free	27121704	1
Fagron	SyrSpend [®] SF pH4 aroma free	17202371	1
Fagron	SyrSpend [®] SF pH4 aroma free	1712023/1	14
Fagron	SyrSpend [®] SF pH4 aroma free	1712023/2	36
Fagron	SyrSpend [®] SF pH4 aroma free	18026531	1
Fagron	SyrSpend [®] SF pH4 aroma free	102653/1	1
Fagron	SyrSpend [®] SF pH4 aroma free	1802653/4	2
Fagron	SyrSpend [®] SF pH4 aroma free	1804245/1	33
Fagron	SyrSpend [®] SF pH4 aroma free	1712023/2/	1
Fagron	SyrSpend [®] SF pH4 aroma free	17122018	1
Fagron	SyrSpend [®] SF pH4 aroma free	18025653/1	1
Fagron	SyrSpend [®] SF pH4 aroma free	1812150/2	19
Fagron	SyrSpend [®] SF pH4 aroma free	18042451	1
Fagron	SyrSpend [®] SF pH4 aroma free	18082062	1
Fagron	SyrSpend [®] SF pH4 aroma free	1808206/	1
Fagron	SyrSpend [®] SF pH4 aroma free	1911010	6
Fagron	SyrSpend [®] SF pH4 aroma free	190114110	1
Fagron	SyrSpend [®] SF pH4 aroma free	20007563	26
Fagron	SyrSpend [®] SF pH4 aroma free	20007561	1
Fagron	SyrSpend [®] SF pH4 aroma free	20007575	16
Fagron	SyrSpend [®] SF pH4 aroma free	21005761	11
Fagron	SyrSpend [®] SF pH4 aroma free	T09-0958908	1
Fagron	SyrSpend [®] SF pH4 aroma free	22D11-T09-095898	36
Fagron	SyrSpend [®] SF pH4 aroma free	22D11T09	1
Fagron	SyrSpend [®] SF pH4 aroma free	22D11-T09	4
Fagron	SyrSpend [®] SF pH4 aroma free	22H30-T05-099074	1
Fagron	SyrSpend [®] SF pH4 aroma free	22D11-T08	5
Fagron	SyrSpend [®] SF pH4 aroma free	21009236	1
Fagron	SyrSpend [®] SF pH4 aroma free	22H11-T09	6
Fagron	SyrSpend [®] SF pH4 aroma free	22d11-t08-095894	1

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Supplier	Substance	Batch	Spectra
Fagron	SyrSpend [®] SF pH4 aroma free	3103124	1
Fagron	SyrSpend [®] SF pH4 aroma free	23809-T05-102908	1
Fagron	SyrSpend [®] SF pH4 aroma free	23>B17-T03-103124	1
Fagron	SyrSpend [®] SF pH4 aroma free	1808206-2	1
Fagron	SyrSpend [®] SF pH4 aroma free	1804245-2	1
Fagron	SyrSpend [®] SF pH4 aroma free	20004219	65
Fagron	SyrSpend [®] SF pH4 aroma free	21009136/2301251	1
Fagron	SyrSpend [®] SF pH4 aroma free	1704493	12
Fagron	SyrSpend [®] SF pH4 aroma free	1802653/1	24
Fagron	SyrSpend [®] SF pH4 aroma free	1808206/2A	1
Fagron	SyrSpend [®] SF pH4 aroma free	1808206/2B	1
Fagron	SyrSpend [®] SF pH4 aroma free	20009273	77
Fagron	SyrSpend [®] SF pH4 aroma free	22H11-T09-099022	34
Fagron	SyrSpend [®] SF pH4 aroma free	23B10-T02-102920	28
Fagron	SyrSpend [®] SF pH4 aroma free	T09-0958908	1
Fagron	SyrSpend [®] SF pH4 aroma free	T08-0958904	1
Fagron	SyrSpend [®] SF pH4 aroma free	22H11-T10-099025	14
Fagron	SyrSpend [®] SF pH4 aroma free	22D11-T08-095894	3
Fagron	SyrSpend [®] SF pH4 aroma free	22D11-T09-095899	1
Fagron	SyrSpend [®] SF pH4 aroma free	23E19-716-105390	1
Fagron	SyrSpend [®] SF pH4 aroma free	23B08-T05-102908	1
Fagron	SyrSpend [®] SF pH4 aroma free	1906126	41
Fagron	SyrSpend [®] SF pH4 aroma free	19911010	1
Fagron	SyrSpend [®] SF pH4 aroma free	518E-07040	1
Fagron	SyrSpend [®] SF pH4 aroma free	22H11T10099025	2
Fagron	SyrSpend [®] SF pH4 aroma free	22092008	2
Fagron	SyrSpend [®] SF pH4 aroma free	22092007	1
Fagron	SyrSpend [®] SF pH4 aroma free	1907122	29
Fagron	SyrSpend [®] SF pH4 aroma free	1808206/2	71
Fagron	SyrSpend [®] SF pH4 aroma free	22000887	28
Fagron	SyrSpend [®] SF pH4 aroma free	1712023/02	1
Fagron	SyrSpend [®] SF pH4 aroma free	19011410	100
Fagron	SyrSpend [®] SF pH4 aroma free	4415A-07040	1
Fagron	SyrSpend [®] SF pH4 aroma free	T09-0958909	1
Fagron	SyrSpend [®] SF pH4 aroma free	1808206/1	3
Fagron	SyrSpend [®] SF pH4 aroma free	1814231	35
Fagron	SyrSpend [®] SF pH4 aroma free	21009136	42
Fagron	SyrSpend [®] SF pH4 aroma free	2009273	2
Fagron	SyrSpend [®] SF pH4 aroma free	22H11-165220	1
Fagron	SyrSpend [®] SF pH4 aroma free	20006608	58
Fagron	SyrSpend [®] SF pH4 aroma free	720024-0003	3
Fagron	SyrSpend [®] SF pH4 aroma free	20004220	21
Fagron	SyrSpend [®] SF pH4 aroma free	1503D009	3
Fagron	SyrSpend [®] SF pH4 aroma free	1802653/2	5
Fagron	SyrSpend [®] SF pH4 aroma free	1802654	13
Fagron	SyrSpend [®] SF pH4 aroma free	18c2653/1	1
Fagron	SyrSpend [®] SF pH4 aroma free	22d11-t09-095898	1
Fagron	SyrSpend [®] SF pH4 aroma free	22D11T05095898	1
Fagron	SyrSpend [®] SF pH4 aroma free	1808206/12	1
Fagron	SyrSpend [®] SF pH4 aroma free	1804245/2	3
Fagron	SyrSpend [®] SF pH4 aroma free	1412D002	3
Gehe	SyrSpend [®] SF pH4 aroma free	23A24-T16-106100	4
Gehe	SyrSpend [®] SF pH4 aroma free	23E19-T16-105390	17
Fagron	SyrSpend [®] SF pH4 aroma free	19011210	1
kehr	SyrSpend [®] SF pH4 aroma free	22H11T09099022	1
kehr	SyrSpend [®] SF pH4 aroma free	23b02t16106339	1

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Supplier	Substance	Batch	Spectra
Kehr	SyrSpend [®] SF pH4 aroma free	23D05-T03-104272	2
Noweda	SyrSpend [®] SF pH4 aroma free	2006608	1
Noweda	SyrSpend [®] SF pH4 aroma free	22D11T09095898/2305020	1
Noweda	SyrSpend [®] SF pH4 aroma free	23E19-T12	4
Phoenix	SyrSpend [®] SF pH4 aroma free	200069608	1
Phönix	SyrSpend [®] SF pH4 aroma free	1802653/01	1
Phönix	SyrSpend [®] SF pH4 aroma free	23810-T02-102920	1
S	SyrSpend [®] SF pH4 aroma free	23B17-t03-103124	1

T

Supplier	Substance	Batch	Spectra
Taoasis	Tolu res. 50% oil	493887-105384	1
Taoasis	Tolu res. 50% oil	546022-114802	2
Taoasis	Tolu res. 50% oil	546022-122636	1
Taoasis	Tolu res. 50% oil	23772-118646	1
Taoasis	Tolu res. 50% oil	23772-119167	1

V

Supplier	Substance	Batch	Spectra
Caelo	Vario base cream	13143401	1
Caelo	Vario base cream	14331902	4
Caelo	Vario base cream	16032402	1
Caelo	Vario base cream	13257102	2
Caelo	Vario base cream	12077902	1
Bombastus	Vario base cream	12375801	1
Phoenix 30.1.2013	Vario base cream	12172501	1
Fagron	Versatile [™]	1503256	1
Fagron	Versatile [™]	14B19-T02-010391	2
Fagron	Versatile [™] Rich	247224-0002	1
Fagron	Versatile [™] Rich	14B19-T04-0130395	1
Fagron	Versatile [™] Rich	1503257	4
Phönix	Versatile [™] Rich	1503258	1

W

Supplier	Substance	Batch	Spectra
	Wart ointment InfectoPharm [®] ...	SQ12301.1	1
	Wart ointment InfectoPharm [®] ...	S,12301.1	1
	Wart ointment InfectoPharm [®] ...	s012301.1	2
	Wart ointment InfectoPharm [®] ...	S052302.1	6
	Wart ointment InfectoPharm [®] ...	s052302.1	1
	Wart ointment InfectoPharm [®] ...	S02302.1	1
	Wart ointment InfectoPharm [®] ...	S012401.1	22
	Wart ointment InfectoPharm [®] ...	S012401	2
	Wart ointment InfectoPharm [®] ...	S012401.1	1
	Wart ointment InfectoPharm [®] ...	s012401.1	5
	Wart ointment InfectoPharm [®] ...	S012401_1	1
	Wart ointment InfectoPharm [®] ...	S082402.1	16
	Wart ointment InfectoPharm [®] ...	s082402.1	1
	Wart ointment InfectoPharm [®] ...	S012501.1	7
	Wart ointment InfectoPharm [®] ...	S0125011	3
	Wart ointment InfectoPharm [®] ...	S01251.1	1
	Wart ointment InfectoPharm [®] ...	S052502.1	1
	Wart ointment InfectoPharm [®] ...	S052502.01	1
	Wart ointment InfectoPharm [®] ...	S01250.11	1
AHD	Wart ointment InfectoPharm [®] ...	S0124011	1

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Supplier	Substance	Batch	Spectra
Caelo	Wart ointment InfectoPharm®...	S111202	2
Caelo	Wart ointment InfectoPharm®...	s0617012	1
Euro OTC	Wart ointment InfectoPharm®...	S011401.1	7
Gehe	Wart ointment InfectoPharm®...	S111202.1	1
Gehe/Infectopharm	Wart ointment InfectoPharm®...	S021601.1	15
Infecto Pharm	Wart ointment InfectoPharm®...	S1111702.1	1
Infecto Pharm / Noweda	Wart ointment InfectoPharm®...	S061701.1	9
infectopharm	Wart ointment InfectoPharm®...	S091302.1	5
infectopharm	Wart ointment InfectoPharm®...	S041402.1	1
infectopharm	Wart ointment InfectoPharm®...	S0211604	1
Infectopharm	Wart ointment InfectoPharm®...	3013I-07003	1
Infectopharm	Wart ointment InfectoPharm®...	S041301.1	4
Infectopharm	Wart ointment InfectoPharm®...	S041301	1
Infectopharm	Wart ointment InfectoPharm®...		2
Infectopharm	Wart ointment InfectoPharm®...	s021501.01	1
Infectopharm	Wart ointment InfectoPharm®...	5061701.1	1
Infectopharm	Wart ointment InfectoPharm®...	S05190.1	1
Infectopharm	Wart ointment InfectoPharm®...	S052101.1	23
Infectopharm	Wart ointment InfectoPharm®...	s052101.1	2
Infectopharm	Wart ointment InfectoPharm®...	s0422.01	1
Infectopharm	Wart ointment InfectoPharm®...	S012301.1	21
InfectoPharm	Wart ointment InfectoPharm®...	S041301,1	1
InfectoPharm	Wart ointment InfectoPharm®...	S091502.1	21
InfectoPharm	Wart ointment InfectoPharm®...	S111702.1	18
InfectoPharm	Wart ointment InfectoPharm®...	s061801	1
InfectoPharm	Wart ointment InfectoPharm®...	S121902.1	41
InfectoPharm	Wart ointment InfectoPharm®...	s112001.1	2
InfectoPharm	Wart ointment InfectoPharm®...	S012301.01	2
Infectopharm (Phoenix)	Wart ointment InfectoPharm®...	S111202.2	3
Infectopharm / Alliance	Wart ointment InfectoPharm®...	S051801.1	1
InfectoPharm / Gehe	Wart ointment InfectoPharm®...	S111702,1	1
Infectopharm / Noweda	Wart ointment InfectoPharm®...	Ch.B.060521/A	1
Infectopharm / Phönix	Wart ointment InfectoPharm®...	4117A-03898	1
Infectopharm / Phönix	Wart ointment InfectoPharm®...	3718A-03898	1
Infectopharm Arzne...	Wart ointment InfectoPharm®...	S111702.01	1
Infectopharm Arzne...	Wart ointment InfectoPharm®...	s061801.1	5
Infectopharm Arzne...	Wart ointment InfectoPharm®...	S112102.1	22
Infectopharm GmbH	Wart ointment InfectoPharm®...	s061801-1	1
Infectopharm Sanacorp	Wart ointment InfectoPharm®...	S061801	1
Infectopharm/ Alliance	Wart ointment InfectoPharm®...	51901.1	1
InfectoPharm/ Gehe	Wart ointment InfectoPharm®...	S051901.01	1
Infectopharm/ Phönix	Wart ointment InfectoPharm®...	s052101.2	1
Infectopharm/AEP	Wart ointment InfectoPharm®...	S112001	1
Infectopharm/AHD	Wart ointment InfectoPharm®...	S1219021	1
infectopharm/Alliance	Wart ointment InfectoPharm®...	S061801.1	32
InfectoPharm/Anzag	Wart ointment InfectoPharm®...	716A-03898	1
Infectopharm/Gehe	Wart ointment InfectoPharm®...	S021501.1	11
Infectopharm/Gehe	Wart ointment InfectoPharm®...	S061701.2	20
Infectopharm/Gehe	Wart ointment InfectoPharm®...	S0617001.2	1
Infectopharm/Gehe	Wart ointment InfectoPharm®...	S112001.1	39
Infectopharm/Gehe	Wart ointment InfectoPharm®...	S112001.01	1
Infectopharm/Gehe	Wart ointment InfectoPharm®...	S052101.2	10
InfectoPharm/Gehe	Wart ointment InfectoPharm®...	S071602.1	15
INFECTOPHARM/GEHE	Wart ointment InfectoPharm®...	S071602:1	1
...			
INFECTOPHARM/GEHE	Wart ointment InfectoPharm®...	s061701.2	1
...			

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Supplier	Substance	Batch	Spectra
Infectopharm/Kehr	Wart ointment InfectoPharm®...	\$042201.1	1
Infectopharm/Nk	Wart ointment InfectoPharm®...	S051901	1
Infectopharm/Nk	Wart ointment InfectoPharm®...	S112001,1	1
Infectopharm/Noweda	Wart ointment InfectoPharm®...	S111403.1	12
Infectopharm/Noweda	Wart ointment InfectoPharm®...	S0716021	1
Infectopharm/Noweda	Wart ointment InfectoPharm®...	S061701.01	2
Infectopharm/Noweda	Wart ointment InfectoPharm®...	S061701,2	1
Infectopharm/Noweda	Wart ointment InfectoPharm®...	S0521011	1
InfectoPharm/Noweda	Wart ointment InfectoPharm®...	S041402.1	4
Infectopharm/Phoenix	Wart ointment InfectoPharm®...	A111702.1	1
Infectopharm/Phoenix	Wart ointment InfectoPharm®...	S042201.1	11
Infectopharm/Phönix	Wart ointment InfectoPharm®...	S051901.1	39
Infectopharm/Phönix	Wart ointment InfectoPharm®...	A121902.1	1
Infectopharm/Phönix	Wart ointment InfectoPharm®...	S052101.1	1
Infectopharm/Römer...	Wart ointment InfectoPharm®...	S0215011	6
Infectopharm/Spangro	Wart ointment InfectoPharm®...	S061801-1	1
Infectopharm	Wart ointment InfectoPharm®...	s051901.1	4
Löwen City-Apothek...	Wart ointment InfectoPharm®...	8032013	1
InfectoPharm	Wart ointment InfectoPharm®...	A041301.1	1
Noweda/infectopharm	Wart ointment InfectoPharm®...	S091502,1	2
Noweda/InfectoPharm	Wart ointment InfectoPharm®...	s021601.1	4
Noweda/InfectoPharm	Wart ointment InfectoPharm®...	S1120001.1	1
Phönix	Wart ointment InfectoPharm®...	S51901.1	3
Phönix	Wart ointment InfectoPharm®...	S051901:1	3
Phönix, Infectopha...	Wart ointment InfectoPharm®...	S129021	1
Taoasis	Wild rose oil	99149-99474	1
Taoasis	Wild rose oil	106177-106175	1

Appendix D: Requirements of validation

In order to ensure adherence to the safe scientific status, the individual methods for manufacturing and testing must be validated under certain circumstances (compare § 34 para. 1 no. 3, § 35 para. 1 no. 4 and para. 4 sentence 1 no. 2 b, para. 6 sentence 3 *ApoBetrO* [Pharmacies Rules and Regulations]). The *ApoBetrO* [Pharmacies Rules and Regulations] incorporates a legal definition in § 1 a para. 16 (quotation translated):

“Validation is the provision of documented proof which with a high degree of safety documents that, via a specific process or standard work process, a medicinal product is manufactured and tested, which is in accordance with previously determined quality features.”

Validation documentation can be used to prove that methods or devices which are not described in the Pharmacopoeia within the meaning of § 6 para. 1 sentence 3 *ApBetrO* [Pharmacies Rules and Regulations] achieve the same results as those in the Pharmacopoeia. On the other hand, with the requirements of the demanded validation it must be observed whether the respective testing method is already incorporated in the Pharmacopoeia.

NIR spectroscopy as a general testing method need not be validated in accordance with the express ruling in the *Ph. Eur. Section 1.1* [3], as it is already described in *Section 2.2.40* of the *Ph. Eur.* as an area of application for the identification of raw materials.

However, a special validation requirement exists for the reference database. This requirement is met with the existing document. Further requirements or rules as to how this proof must be furnished do not exist. It is required that the processes guarantee the same results as the methods and devices in the Pharmacopoeia [17].

Carrying out identity tests with *Apo-Ident* is therefore also possible if the NIR spectroscopy process is not required in the Pharmacopoeia monograph of the substance for identity testing. All NIR analyses with *Apo-Ident* prove several, often all molecule groups and are therefore comparable with a series of individual, targeted chemical proofs [4]. Therefore, the identity proof with *Apo-Ident* replaces the monograph test series (with two or more test combinations).

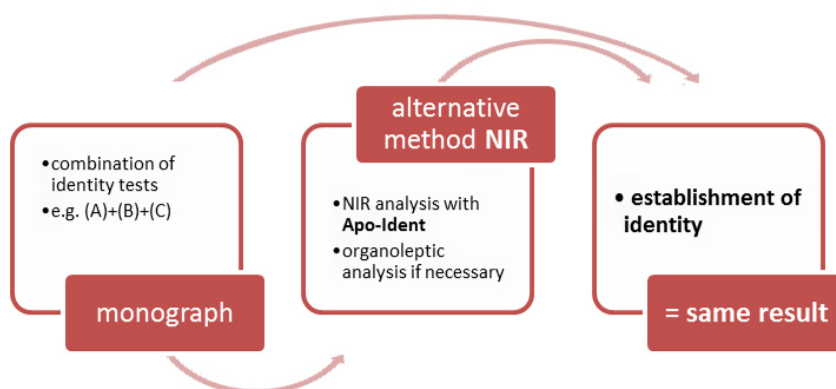


Figure 2: The combination of tests of the monograph is replaced by the alternative method NIR spectroscopy using *Apo-Ident*. This is permissible because both test procedures result in the establishment of the identity of the raw material.

With this validation documentation, proof is furnished that identical results are achieved with *Apo-Ident* and Pharmacopoeia methods, i.e. confirmation of the identity of the raw material [2].

Appendix E: Conformity of Apo-Ident with the European pharmacopeia

According to *Ph. Eur. Section 2.2.40*, NIR spectroscopy is basically suitable for: “Identification of agents, excipients, dosage forms, intermediate manufacturing products, chemical raw materials and packaging materials” ([3], quotation translated).

The fact that *Apo-Ident* meets the further criteria of the European Pharmacopoeia under the headings in *Section 2.2.40*

- Apparatus
- Measurement methods
- Sample preparation and presentation
- Testing the functionality of the instrument
- Identification and characterisation (qualitative analysis)
- Quantitative analysis
- Ongoing model evaluation
- Transfer of databases
- Data storage

can be proven based on the *HiperScan GmbH* documentation of “Meeting 2.2.40 *Ph. Eur.* by *Apo-Ident*” [4].

Appendix F: Explanation of the spectrum acquisition under the control of HiperScan GmbH

The spectra for the generation of the database (*type A*) and the spectra for the validation of the database (*type B*) are recorded exclusively under the control of *HiperScan GmbH*. This means that the spectra are recorded either by a qualified employee of *HiperScan GmbH* or by an employee of the *Fagron Group* who has been trained and authorised by *HiperScan GmbH*. Prior to inclusion in the database, the quality assurance of the spectra is carried out by a qualified employee of *HiperScan GmbH*.

Appendix H: Module for Qualitative Analysis of Cannabis Flowers

The qualitative analysis of cannabis flowers is available only to subscribers of the corresponding reference database. This enables the use of an additional module as a second-stage model.

Purpose of the Module

The module provides evidence of the presence of both Δ^9 -tetrahydrocannabinol (THC) and cannabidiol (CBD), as well as their acid forms, in cannabis flowers and essential oil-containing herbal drugs (e.g., hop strobiles, rosemary leaves, mate leaves, peppermint leaves, and many others). A result is considered positive if the mass fraction is at least 5 %.

A qualitative detection of THC and/or CBD is carried out using qualitative methods in accordance with *Ph. Eur. Section 5.21 Chemometric methods for the evaluation of analytical data*. Thus, the module for the qualitative analysis of cannabis flowers represents, in most cases, a complete alternative to the thin-layer chromatography (TLC) method described in the monograph for cannabis flowers. In cases where the module cannot deliver a fully reliable result, the use of another validated analytical method is recommended (see *Structure and Functionality*).

Structure and Functionality

The spectrum of a cannabis flower undergoes the following steps within the IdentModule:

1. Upon selecting one of the three chemotypes of cannabis flowers, the sample spectrum is first analyzed using the model for *Solid APIs & excipients*.
2. If one of the three cannabis chemotypes is identified as the closest match in the *Solid APIs & excipients* model, the spectrum is forwarded to the module for qualitative analysis of cannabis flowers.
3. The spectrum is checked for similarity to known cannabis flower spectra. This test may also be passed for spectra from other essential oil-containing herbal drugs. Fundamentally dissimilar spectra are rejected at this stage.
4. The sample is analyzed in parallel using two specialized models that yield a positive or negative result for THC and/or CBD detection. If the model cannot provide a clearly reliable result (e.g., if cannabinoid content is near the 5 % threshold), a neutral result is returned.
5. Based on the results of the THC and CBD models, the substance is identified as follows:

Model Result for		
THC	CBD	Substance
positive	positive	Cannabis flower, THC/CBD type
positive	negative	Cannabis flower, THC type
negative	positive	Cannabis flower, CBD type
negative	negative	Sample rejected, as it cannot be a defined and selectable medicinal substance
neutral	(...)	Recommendation to conduct another validated analysis, e.g.,
(...)	neutral	TLC

6. Finally, the result is compared with the initial assumption (selected substance).

Cannabis Flower Substances and Samples

For model development and module optimization, cannabis flowers of pharmaceutical quality were primarily used. These cover the full range of THC/CBD content combinations available in pharmacies. The quality of these flowers is documented through appropriate manufacturer certificates. Additionally, CBD-type flowers from so-called CBD shops were recorded to supplement the data base. These samples mainly serve to improve model robustness and have limited relevance to the pharmacy market. Certificates are only partially available for these samples.

The THC and CBD content of all cannabis flower samples was determined via HPLC, in accordance with the valid monograph, using the same flower(s) from which the NIR spectra were obtained. The date of this analysis is listed in the validation report tables under *Certificate*. Based on these reference values, samples were classified as THC- or CBD-containing if the content (mass fraction) exceeded the 5 % threshold. Subsequently, the samples were grouped into substances by chemotype in accordance with point 5 of the table under *Structure and Functionality*.

- The following samples exhibit a THC content above and a CBD content below 5 %. They have been assigned to the *THC-dominant chemotype*.

Sample ID	Producer	Brand	Content / %	
			THC	CBD
B10001	Weeco Pharma	1A 18/1 Weeco	13.91	0.07
B10002	Four 20 Pharma	420 Evolution 25/1 CA ICC	24.07	0.10
B10003	Four 20 Pharma	420 Evolution 27/1 CA ICC	25.65	0.12
B10004	Four 20 Pharma	420 Evolution 27/1 CA WES	26.21	0.14
B10005	Four 20 Pharma	420 Natural 22/1 CA GG4	22.30	0.09
B10006	Four 20 Pharma	420 Natural 27/1 CA ZRP	22.87	0.10
B10007	ADREXpharma	Adrex 17/1 CAN	13.37	0.09
B10008	ADREXpharma	Adrex 22/1 CAN	22.04	0.11
B10009	AMP	AMP Classic 18/1	17.63	0.08
B10010	AMP	AMP Classic 25/1	23.23	0.10
B10012	Aurora Deutschland	Aurora 20/1 DNK	18.13	0.14
B10013	Aurora Deutschland	Aurora 22/1 DNK	16.93	0.11
B10014	Canopy Growth Corporation	Bakerstreet 20	21.75	0.08
B10015	Bedrocan International B.V.	Bedica	13.43	0.12
B10017	Bedrocan International B.V.	Bedrocan	16.48	0.15
B10019	Canopy Growth Corporation	Canopy AKH 22	24.66	0.13
B10021	Canopy Growth Corporation	Canopy Krypton 25	25.52	0.12
B10022	Canopy Growth Corporation	Canopy LSK 16	18.75	0.12
B10023	Tilray Deutschland	Navcora THC22 Porto	19.65	0.10
B10024	Tilray Deutschland	Navcora THC22 Porto	18.35	0.11
B10025	Aurora Deutschland	Pedanos 20/1 DNK	18.63	0.09
B10026	Aurora Deutschland	Pedanos 22/1 DNK	23.98	0.12
B10027	Aurora Deutschland	Pedanos 27/1 FRG-CA	27.67	0.17
B10028	Aurora Deutschland	Pedanos 29/1 SRD-CA	30.07	0.14
B10029	Pharmcann Deutschland	Pharmcann Silver THC22	22.95	0.18
B10030	Fette Pharma	RE:CANNIS Blüten 16/1 Sativa	12.76	0.07
B10031	Fette Pharma	RE:CANNIS Blüten 21/1 Indica	20.34	0.13
B10033	Remexian Pharma	Remexian 22/1	21.89	0.35
B10034	Remexian Pharma	Remexian 25/1	21.05	0.12
B10035	Remexian Pharma	Remexian 25/1 GAC	22.55	0.10
B10036	WMG Pharma	Supreme 24/1 WMG Pharma	24.12	0.11
B10038	Tilray Deutschland	Tilray THC18 Spotlight Porto	12.63	0.31
B10039	Tilray Deutschland	Tilray THC18 Spotlight Porto	13.89	0.08
B10040	Tilray Deutschland	Tilray THC22 Indica No. 2	16.41	0.10
B10041	Tilray Deutschland	Tilray THC22 Montevideo	17.02	0.08
B10042	Tilray Deutschland	Tilray THC22 Sativa No. 2	19.94	0.09
B10043	Tilray Deutschland	Tilray THC25 Montevideo	22.32	0.11
B10044	Tilray Deutschland	Tilray THC25 Sativa No. 2	17.42	0.10
B10045	Tilray Deutschland	Tilray THC25 Spotlight Porto	19.08	0.12
B10046	Tilray Deutschland	Tilray THC25 Spotlight Porto	20.17	0.10
B10047	Tilray Deutschland	Tilray THC25 Spotlight Porto	17.16	0.07
B10048	Tilray Deutschland	Tilray THC25 Spotlight Porto	19.31	0.09
B10049	Tilray Deutschland	Tilray THC25 Spotlight Porto	20.14	0.12
B10050	Tilray Deutschland	Tilray THC22 Spotlight Porto	19.51	0.09
B10051	Tilray Deutschland	Tilray THC22 Spotlight Porto	15.71	0.09

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Sample ID	Producer	Brand	Contant / %	
			THC	CBD
B10052	Tilray Deutschland	TilrayTHC22 Spotlight Porto	20.61	0.10
B10053	Vayamed	Vayamed 22/1	20.76	0.19
B10054	Weeco Pharma	Weeco 23/1	23.63	0.11
B10055	Weeco Pharma	Weeco 25/1	22.66	0.11
B10057	Four 20 Pharma	420 Evolution 27/1 CA STR	23.78	0.51
B10058	Four 20 Pharma	420 Natural 17/1 CA TRP	18.26	0.11
B10059	Four 20 Pharma	420 Natural 20/1 CA GG4	21.94	0.10
B10060	ADREXpharma	Adrex 30/1 8BK CAN	30.29	0.15
B10061	ADREXpharma	Adrex 26/1 AK COL	24.45	0.15
B10062	Cansativa	AMICI SB 29/1	23.91	0.10
B10064	Vayamed	Avaay 23/1 CK Critical Kush	18.58	0.29
B10065	WMG Pharma	Supreme 18/1 WMG	15.28	0.11
B10089	Four 20 Pharma	420 Evolution 27/1 CA ICC	25.36	0.32
B10090	Four 20 Pharma	420 Evolution 27/1 CA WES	27.11	0.15
B10091	Four 20 Pharma	420 Natural 27/1 CA ZRP	24.02	0.11
B10092	ADREXpharma	Adrex 17/1 CAN	13.75	0.09
B10098	Canopy Growth Corporation	Canopy LSK 16	19.72	0.29
B10099	Aurora Deutschland	Pedanos 27/1 FRG-CA	25.77	0.19
B10100	Aurora Deutschland	Pedanos 29/1 SRD-CA	30.81	0.15
B10101	Fette Pharma	RE:CANNIS Blüten 16/1 Sativa	13.27	0.08
B10104	Weeco Pharma	Weeco 25/1	23.95	0.20
B10106	Four 20 Pharma	420 Evolution 27/1 CA STR	27.95	0.13
B10107	Four 20 Pharma	420 Natural 17/1 CA TRP	18.54	0.10
B10108	ADREXpharma	Adrex 30/1 8BK CAN	29.25	0.15
B10109	ADREXpharma	Adrex 26/1 AK COL	27.62	0.20
B10110	Cansativa	AMICI SB 29/1	26.73	0.15
B10117	Canopy Growth Corporation	Canopy LSK 16	10.59	0.16
B10118	Aurora Deutschland	Pedanos 29/1 SRD-CA	29.59	0.18
B10119	Fette Pharma	RE:CANNIS Blüten 16/1 Sativa	15.73	0.17
B10123	ADREXpharma	Adrex 30/1 8BK CAN	27.28	0.19
B10124	Cansativa	AMICI SB 29/1	26.47	0.13
B10126	Weeco Pharma	1A 18/1 Weeco	17.19	0.11
B10127	AMP	AMP Classic 18/1	17.93	0.10
B10128	Tilray Deutschland	Tilray THC18 Spotlight Porto	11.60	0.06
B10129	Tilray Deutschland	Tilray THC18 Spotlight Porto	15.24	0.09
B10130	Aurora Deutschland	Pedanos 27/1 FRG-CA	27.21	0.18
B10131	Four 20 Pharma	420 Evolution 27/1 CA STR	26.86	0.10

- The following samples exhibit both THC and CBD contents above 5 %. They have been assigned to the *THC/CBD intermediate type*.

Sample ID	Producer	Brand	Contant / %	
			THC	CBD
B20016	Bedrocan International B.V.	Bediol	5.01	7.45
B20020	Canopy Growth Corporation	Canopy HSK 8/7	8.38	7.02
B20032	Fette Pharma	RE:CANNIS Blüten 9,5/10,5 Hybrid	10.52	10.65
B20037	Tilray Deutschland	Tilray 9/9 No.2	9.02	8.46
B20063	Aurora Deutschland	Cannabis Pedanos 8/8	8.33	8.74
B20097	Canopy Growth Corporation	Canopy HSK 8/7	7.95	6.99
B20102	Fette Pharma	RE:CANNIS Blüten 9,5/10,5 Hybrid	9.08	10.08
B20103	Tilray Deutschland	Tilray 9/9 No.2	8.78	8.82
B20111	Aurora Deutschland	Cannabis Pedanos 8/8	8.06	9.17
B20116	Canopy Growth Corporation	Canopy HSK 8/7	7.46	6.23

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Sample ID	Producer	Brand	Contant / %	
			THC	CBD
B20120	Fette Pharma	RE:CANNIS Blüten 9,5/10,5 Hybrid	10.11	10.68
B20121	Tilray Deutschland	Tilray 9/9 No.2	8.22	7.25
B20125	Aurora Deutschland	Cannabis Pedanios 8/8	7.73	8.35
B20140	Cannamedical Pharma	Cannamedical Balanced light	5.38	9.76
B20142	Bedrocan International B.V.	Bediol	6.33	9.56
B20143	Tilray Deutschland	Tilray THC9:CBD9 No.2	9.26	9.94
B20144	Aurora Deutschland	Pedanios 10/13 MBE-CA	9.22	14.17
B20145	Aurora Deutschland	Pedanios 10/10 EQI-CA	10.10	11.60
B20154	IMC (Adjupharm)	IMC balanced 7/8 B01	8.43	9.36

- The following samples exhibit a THC content below and a CBD content above 5 %. They have been assigned to the *CBD-dominant chemotype*.

Sample ID	Producer	Brand	Contant / %	
			THC	CBD
B30011	Aurora Deutschland	Aurora 1/12 DNK	0.56	13.14
B30018	Bedrocan International B.V.	Bedrolite	0.24	6.32
B30056	Fette Pharma	RE:CANNIS Blüten 1/15	1.40	14.53
B30073	Ecommerce Space	Sieved Mix Indoor	0.14	5.00
B30077	Lucky Life	Strawberry Aroma	0.15	5.47
B30080	bubatzbros.de	Cali Essentials "California Dream"	0.68	16.50
B30081	bubatzbros.de	Cali Essentials "Mango Kush"	0.58	11.69
B30083	HGV Kräutergarten	Tropical Haze Outdoor CBD Blüten	0.39	11.87
B30084	HGV Kräutergarten	Sweet Babe Blüten	0.19	5.22
B30085	HGV Kräutergarten	Blue Bear OG Premium Blüten	0.09	5.64
B30086	HGV Kräutergarten	Northern Lights Premium CBD-Blüten	0.49	14.78
B30087	HGV Kräutergarten	Purple Haze Premium Blüten	0.17	5.47
B30088	HGV Kräutergarten	White Widow Premium Blüten	0.07	6.78
B30093	Aurora Deutschland	Aurora 1/12 DNK	0.59	11.75
B30105	Fette Pharma	RE:CANNIS Blüten 1/15	1.02	15.84
B30112	Aurora Deutschland	Aurora 1/12 DNK	0.58	12.48
B30122	Fette Pharma	RE:CANNIS Blüten 1/15	0.93	16.07
B30132	CBD NOL	CBD Blüten Premium - Redwood Kush	0.18	5.09
B30135	CBD NOL	CBD Blüten Premium - Purple Kush	0.32	8.98
B30146	CBD Express	Gelato	0.10	6.97
B30147	CBD Express	Skywalker OG	0.26	10.94
B30149	CBD Express	Cameleon	0.14	7.53
B30150	CBD Express	Harlequin	0.07	10.53

- The following samples exhibit both THC and CBD contents below 5 %. They do not correspond to any cannabis flower chemotype according to the monograph, but were included in the model for demarcation purposes, similar to essential oil-containing herbal drugs.

Sample ID	Producer	Brand	Contant / %	
			THC	CBD
B40066	Malkmus Holistic	Space Grown Orbitz by Marvin Game	0.47	2.76
B40067	Malkmus Holistic	Mexican Gold	0.07	2.18

continued on following page

Sample ID	Producer	Brand	Contant / %	
			THC	CBD
B40068	Malkmus Holistic	Cherry Calussi	0.12	3.31
B40069	Malkmus Holistic	Melon Kush Deluxe	0.06	2.70
B40070	Malkmus Holistic	Sweet Berry Jane	0.01	2.02
B40071	Malkmus Holistic	Bubba Berry by AchtVier	0.12	3.15
B40072	Malkmus Holistic	Super Lemon Haze 15% CBD	0.00	1.47
B40074	Ecommerce Space	Sweet Berry	0.08	3.25
B40075	Ecommerce Space	Gorilla Glue	0.15	4.74
B40076	Lucky Life	California Blueberry	0.02	2.61
B40078	Lucky Life	Orange Bud	0.00	1.68
B40079	Lucky Life	Purple Touch	0.13	4.01
B40082	HGV Kräutergarten	Lennon Haze CBD Blüten	0.08	4.14
B40133	CBD NOL	CBD Blüten Premium - Super Lemon Haze	0.04	2.18
B40134	CBD NOL	CBD Blüten - Cannatonic	0.06	3.51
B40136	CBD NOL	CBD Blüten - Amnesia Haze	0.12	4.17
B40137	CBD NOL	CBD Blüten - Pineapple Express	0.20	4.46
B40138	CBD NOL	CBG Blüten Premium - Big Bud	0.09	0.12
B40139	CBD NOL	CBD Blüten Premium - Bel Air	0.19	2.84
B40141	Vayamed	avaay 5/1 THCV12	3.74	0.10
B40148	CBD Express	CBN Blüten V-One	0.16	4.77

Each of these cannabis flowers was first measured with the Apo-Ident directly as taken from the package, without any pretreatment. Subsequently, spectra of ground flowers were also recorded. This approach is intended to increase the robustness of the model.

Unambiguous Identifiability

A [specificity](#) of 100 % ([true negative rate](#)) is required for the module for qualitative analysis of cannabis flowers.

In contrast to other models, the distance to other substances is not evaluated directly. Instead, a probability value for a positive or negative result is calculated based on *Type A* spectra within a given distance from the sample spectrum. From all available cannabis flower samples, a threshold was determined for correct identifications. If the probability value of the sample exceeds this threshold plus a safety margin, the identification is considered unambiguous. Otherwise, a neutral result is issued. The probability thresholds used are summarized in the following table:

Model	Classification	Probability Threshold
CBD Identification	CBD positive	0.92
	CBD negative	0.82
THC Identification	THC positive	0.89
	THC negative	0.85

Validation and Scope of the Models

The detection of THC and CBD, including their acid forms, is performed using two specialized PCA models. These are trained with spectra of cannabis flowers, pure cannabinoids, and selected herbal drugs.

To define the herbal drug selection, all pharmacy-relevant herbal drugs were initially considered together with cannabis flowers using the main model for *Solid APIs & excipients*. Herbal drugs whose spectral distance to cannabis flower samples was smaller than the distance to the next API were selected. After building the first generation of the THC and CBD models, the herbal drugs with the largest spectral distance to cannabis flower samples were successively removed until no further improvement in detection rate could be achieved.

The module for qualitative analysis of cannabis flowers is implemented as a second-stage model following the model for *Solid APIs & excipients* (analogous to the submodels). The main model acts as a prefilter, ensuring that only spectra similar to cannabis flower spectra are forwarded. This applies to cannabis flower spectra and certain essential oil-containing herbal drugs.

The restricted selection of substances for model calibration enables high performance, allowing even subtle spectral differences to be effectively evaluated. In combination with the prefiltering main model, this enables differentiation from a wide range of substances.

The module for qualitative analysis of cannabis flowers has been fully validated against all substances of the classes *Solid APIs & excipients*, *Solid Narcotic Substances*, *Drugs*, and other *Chemicals*.

Ongoing Model Maintenance

According to *Ph. Eur.* [3], regular acquisition of new samples and re-evaluation of chemometric models is required. This necessitates batch maintenance for the cannabis flower analysis module. This also applies to the herbal drugs used for calibrating the PCA models for THC and CBD identification. The spectra of all other herbal drugs are considered sufficiently distinct (correlation < 0.86) from cannabis flower spectra and are thus filtered out beforehand, meaning they are not evaluated by the cannabinoid identification models.

Regular batch maintenance for calibration and validation of the cannabis flower analysis module is performed for the following herbal drugs:

- Nettle seeds
- Herniaria
- Cannabis flowers
- Bitter fennel
- Cloves
- Ginkgo leaves
- Hop strobiles
- Chamomile flowers
- Caraway
- Lavender flowers
- Mate leaves
- Lemon balm leaves
- Pepper
- Peppermint leaves
- Marigold flowers
- Rosemary leaves
- Celery fruits
- Black mustard seeds
- Senna leaflets
- Thyme

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