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

HiperScan GmbH

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Validation documentation of the chemometrics database of the near-infrared spectrometer *Apo-Ident*.
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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-intense, time-intense 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 transflection.
- 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 *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 *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 by *HiperScan GmbH* on traceable samples in pharmaceutical quality.
  - 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.

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- 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.

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)* and *narcotics - solid medicinal substances*. 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. Bezugsquellennachweis 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) Überprüfen der Abstände zwischen den Grenzen der trennbaren Substanzen: Die Distanzmatrix enthält die *Mahalanobis-Abstände* von jeder Substanz zu jeder anderen. Die Werte hin und zurück sind jeweils unterschiedlich, weil die Streuung der Ausgangssubstanz eingeht. Ist eine Distanz kleiner als der Mindestabstand, so gelten die Substanzen als nicht sicher trennbar. Der Mindestabstand ist auf 9 festgelegt. Der Entwickler des Modells darf einen größeren Mindestabstand festlegen (ein Wert für das gesamte *chemometrische Modell*), um die Trennschärfe zu erhöhen.

e) Überprüfung des Modells anhand der Referenzspektren. Es sind keine *falsch-positiven* Ergebnisse erlaubt.

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f) Wird eines der Kriterien verletzt (d) *Unterschrittener Mindestabstand zwischen zwei Substanzen* oder (e) *Eine Substanz wird als eine andere identifiziert*, entscheidet der Entwickler der Datenbank, welche der folgenden Optionen er anwendet:

- Er nimmt beide Substanzen aus der Datenbank. (Die Spektren bleiben in der Validierung und dürfen auch in den Aufbau eingehen. Sie werden aber nicht zur Prüfung angeboten.)
- Er bildet eine Substanzgruppe mehrerer nicht sicher trennbarer Substanzen. Dann ist das Ergebnis mehrdeutig: Das chemometrische Modell stellt fest, dass es sich bei der Probe um eine der Substanzen aus der Gruppe handelt und dass es sich um keine andere Substanz handelt. Es kann aber nicht sagen, um welche der Substanzen es sich handelt. Um die eindeutige Identität festzustellen, muss der Anwender eine geeignete ergänzende Prüfung durchführen.
- Er erstellt ein weiteres *chemometrisches Modell* mit geringerem Umfang, in das mindestens alle Substanzen der nicht sicher trennbaren Substanzgruppe eingehen (Zweite-Stufe-Modell). Zweite-Stufe-Modelle werden nur aufgerufen, wenn die erste Stufe festgestellt hat, dass es sich nur um eine der Substanzen handeln kann, die in den Aufbau der Zweiten Stufe eingegangen ist.

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 *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 a 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)** and **Narcotic substances, liquid/semi-solid**. 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 by *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.

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.

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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 Pharmacopeia* 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-

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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

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

[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 $\mathbf{X}$.

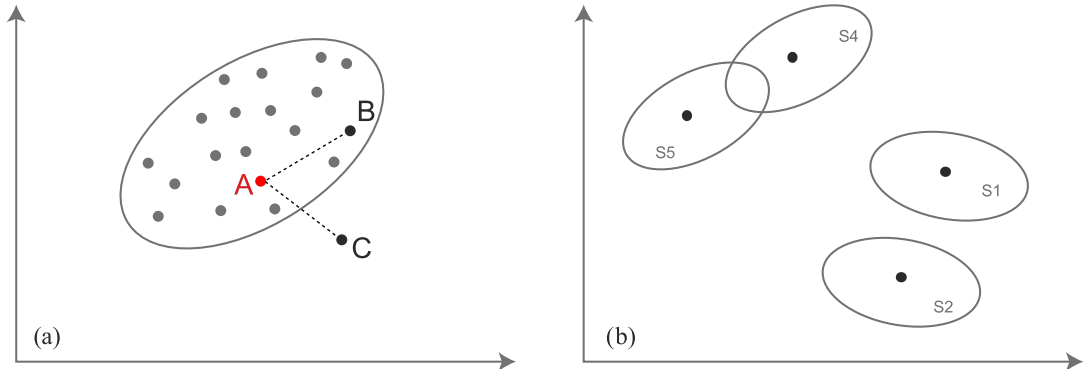

Figure 1: (a) The *Mahalanobis distance* from A to B is less than from A to C. However, the Euclidean distances are identical. (b) The *Mahalanobis distance* between the two measurement series *S4* and *S5* is smaller than between *S1* and *S2*. However, the Euclidean distances are identical.

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.

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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 by *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 70 089 spectra from 6093 different batches for a total of 214 substances were used to validate the substance class *APIs & excipients, liquid/semi-solid (other)*.

Validation samples

The validation samples can be categorised as follows:

Typ A Calibration spectra. These are the spectra used to generate the chemometric model. They were recorded by *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)	160	607	28 555

From category *A* a total of 28 555 spectra from 607 batches for a total of 160 substances were taken into account for validation.

Typ B Spectra from independent samples which are not included in database generation. These spectra were recorded by *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)	210	588	26 101

From category *B* a total of 26 101 spectra from 588 batches for a total of 210 substances were taken into account for validation.

Typ 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)	159	5122	15 433

From category *C* a total of 15 433 spectra from 5122 batches for a total of 159 substances were taken into account for validation.

Validation results

The validation runs checked whether all substances/substance groups in the substance class *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 *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	28 465	0	2 855 590
Type B	0	20 113	938	2 613 199
Type C	0	14 578	372	1 543 544

All substances/substance groups in the substance class *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
Typ A	100.000 00 % (> 99.999 64 %)	100.000 00 % (> 99.965 37 %)
Typ B	100.000 00 % (> 99.999 51 %)	93.188 44 % (> 93.157 50 %)
Typ C	100.000 00 % (> 99.989 85 %)	95.538 48 % (> 95.007 74 %)

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Alfason Basis Cresa®**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30723-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Alfason Basis Cresa®

Special notes

When selecting the *Alfason Basis Cresa®* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Alfason Basis Cresa®	6	1	51

Second-stage model

For differentiation of the substance/substance group *Alfason Basis Cresa*® the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Alfason Basis Cresa*®:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Astellas Pharma	Alfason Basis Cresa®	12B11/77	30723	54	not required
Astellas Pharma	Alfason Basis Cresa®	13D06/75	31071	40	not required
Astellas Pharma	Alfason Basis Cresa®	15I46/79	32064	60	not required
Astellas Pharma	Alfason Basis Cresa®	16D35/77	32815	40	not required
Karo Pharma G…	Alfason Basis Cresa®	20I48/79	35477	40	not required
Karo Pharma G…	Alfason Basis Cresa®	21K41/77	36757	40	not required

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 274 spectra of 6 reference samples from the substance/substance group *Alfason Basis Cresa*®. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 28 281 spectra from a total of 598 batches from further 159 substances. These spectra were recorded by *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 by *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 *Alfason Basis Cresa*®.

- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
LEO Pharma GmbH	Alfason Basis Cresa®	17B27/75	33487	40
Astellas Pharma	Alfason Basis Cresa®	16D35/77	32840	40

- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 93 spectra from 27 *Apo-Ident* customers from 53 batches from the substance/substance group *Alfason Basis Cresa®*.

- Among them are spectra of independent samples from 51 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
A.H.D.	Alfason Basis Cresa®	12/05/75	1
AHD	Alfason Basis Cresa®	13A18/76	1
AHD	Alfason Basis Cresa®	14J02/77	2
Alfason/Gehe	Alfason Basis Cresa®	161J31/75	1
Alfason/krieger	Alfason Basis Cresa®	17F10/76	1
anzag	Alfason Basis Cresa®	18I13/76	2
Astellas / Anzag	Alfason Basis Cresa®	15J3/79	1
Astellas / Noweda	Alfason Basis Cresa®	14J02/77	1
Astellas / Noweda	Alfason Basis Cresa®	15D11/79	2
Astellas / Noweda	Alfason Basis Cresa®	15D1179	1
Astellas / Noweda	Alfason Basis Cresa®	15J35/76	1
Astellas Pharma GmbH/ A...	Alfason Basis Cresa®	16D35/77	1
Astellas Pharma GmbH	Alfason Basis Cresa®	16H03/76	1
Astellas Pharma/Noweda	Alfason Basis Cresa®	15J38/79	1
Astellas Pharma	Alfason Basis Cresa®	13K15/75	2
Astellas Pharma	Alfason Basis Cresa®	14C32/78	1
Astellas Pharma	Alfason Basis Cresa®	15D11/79	3
Astellas Pharma	Alfason Basis Cresa®	15H06/80	1
Astellas Pharma	Alfason Basis Cresa®	15J38/79	1
Astellas Pharma	Alfason Basis Cresa®	16A06/76	1
Astellas/Alliance	Alfason Basis Cresa®	15H06/80	1
Astellas/Alliance	Alfason Basis Cresa®	15J35/75	1
Astellas/Alliance	Alfason Basis Cresa®	16J31/75	1
Astellas/Gehe	Alfason Basis Cresa®	14C32/78	1
Astellas/Gehe	Alfason Basis Cresa®	15B14/76	1
Astellas/Gehe	Alfason Basis Cresa®	16G03/75	1
Astellas/Gehe	Alfason Basis Cresa®	20A14/75	2
Astellas/Sanacorp	Alfason Basis Cresa®	19D65/76	3
Astellas/Sanacorp	Alfason Basis Cresa®	19D65/78	1
Astellas	Alfason Basis Cresa®	13A16/76	1
Astellas	Alfason Basis Cresa®	14c32-78	1
Astellas	Alfason Basis Cresa®	14J02/77	1
AStellas	Alfason Basis Cresa®	14J02/77	1
Caelo	Alfason Basis Cresa®	15J35/75	1
Caelo	Alfason Basis Cresa®	17017/76	1
Caelo	Alfason Basis Cresa®	17EB/75	1

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Supplier	Substance	Batch	Spectra
Caelo	Alfason Basis Cresa®	17EB2/75	1
Caeo/Noweda	Alfason Basis Cresa®	15H06/80	1
devesa/Phönix	Alfason Basis Cresa®	17F08/76	2
Ichtyol/Phönix	Alfason Basis Cresa®	13E08/75	1
Karo Pharma AB	Alfason Basis Cresa®	20A14/75	1
Karo Pharma	Alfason Basis Cresa®	20A13/75	1
Karo Pharma	Alfason Basis Cresa®	21C63/75	3
Karo pharma	Alfason Basis Cresa®	21K41/77	1
KaroPharma/Gehe	Alfason Basis Cresa®	20A13/75	1
karoPharma/Gehe	Alfason Basis Cresa®	21K40/75	1
KaroPharma/Sana	Alfason Basis Cresa®	21LD2/75	3
Lamotte/ Noweda	Alfason Basis Cresa®	16A06/76	2
Leo- Pharm	Alfason Basis Cresa®	18D19/76	1
LEO Pharma / Alliance H...	Alfason Basis Cresa®	17F20/76	1
LEO Pharma / Noweda	Alfason Basis Cresa®	17EB2/75	2
LEO Pharma / Noweda	Alfason Basis Cresa®	18D20/75(3x350g)	1
Leo Pharma A/S	Alfason Basis Cresa®	19D88/75	1
Leo Pharma/Gehe	Alfason Basis Cresa®	18A29/75	1
Leo Pharma/Gehe	Alfason Basis Cresa®	18F30/75	1
LEO Pharma/Gehe	Alfason Basis Cresa®	19D87/75	1
Leo Pharma/Phönix	Alfason Basis Cresa®	19D87/75	1
LEO Pharma	Alfason Basis Cresa®	17B27/75	1
Leo Pharma	Alfason Basis Cresa®	19D65/76	1
LEO/Alliance Healthcare	Alfason Basis Cresa®	18D19/76	1
Leo/Alliance	Alfason Basis Cresa®	18D20/75	2
Leo/Gehe	Alfason Basis Cresa®	17C17/76	1
Leo/Gehe	Alfason Basis Cresa®	17F44/76	1
Leo/Gehe	Alfason Basis Cresa®	18J36/75	1
Leo/Noweda	Alfason Basis Cresa®	18K01/77	1
Leo/Phönix	Alfason Basis Cresa®	18A29/75	1
Leopharm/AEP	Alfason Basis Cresa®	17EB3/75	2
Leopharm/Alliance hc	Alfason Basis Cresa®	18D20/75	2
Leopharma/phoenix	Alfason Basis Cresa®	17F46/76	2
Noweda-Astella	Alfason Basis Cresa®	15A01/79	1
Sanacorp	Alfason Basis Cresa®	12F23/76	1
Sanacorp	Alfason Basis Cresa®	13A16/76	1
Sanacorp	Alfason Basis Cresa®	13E08/75	1

- 15 340 spectra from 1164 *Apo-Ident* customers from a total of 4971 batches from a further 158 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 *Alfason Basis Cresa®* 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 *Alfason Basis Cresa®* 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	274	0	28 281
Type B	0	80	0	26 017
Type C	0	92	1	15 338

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The substance/substance group *Alfason Basis Cresa®* 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 % (> 99.9637 %)	100.0000 % (> 97.8102 %)
Type B	100.0000 % (> 99.9508 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9563 %)	98.9247 % (> 95.6989 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Alfason Basis Cresa®* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Neribas® ointment	16.75	–
Alfason® Repair	17.64	–
Asche Basis® ointment	24.12	–
Bepanthen® Wund- und Heilsalbe	32.43	–
Dermatop® base ointment	50.95	–

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

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
30723	30723	0.00	20.90
31071	31071	0.00	19.41
32064	32064	0.00	24.46
32815	32815	0.00	17.64
35477	35477	0.00	27.05
36757	36757	0.00	25.29

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Alfason® Repair**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30724-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Alfason® Repair

Special notes

When selecting the *Alfason® Repair* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Alfason® Repair	6	1	16

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Alfason® Repair*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Astellas Pharma	Alfason® Repair	12F18/77	30724	55	not required
Astellas Pharma	Alfason® Repair	13E16/76	31069	40	not required
Astellas Pharma	Alfason® Repair	16G60/75	32993	40	not required
Karo Pharma G…	Alfason® Repair	20G23/77	35476	40	not required
Karo Pharma G…	Alfason® Repair	22H11A	36758	40	not required
LEO Pharma GmbH	Alfason® Repair	17E20/75	33790	40	not required

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 255 spectra of 6 reference samples from the substance/substance group *Alfason® Repair*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 28 300 spectra from a total of 598 batches from further 159 substances. These spectra were recorded by *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 by *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 *Alfason® Repair*.
- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Astellas Pharma	Alfason® Repair	15K07/77	32562	40

- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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.

- 19 spectra from 4 *Apo-Ident* customers from 16 batches from the substance/substance group *Alfason® Repair*.
- 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
Astellas	Alfason® Repair	13H02/76	1
Astellas	Alfason® Repair	15J09/75	1
GEHE	Alfason® Repair	17J11/79	1
GEHE	Alfason® Repair	17J13/76	1
GEHE	Alfason® Repair	17K83/75	1
GEHE	Alfason® Repair	18EB5/75	1
GEHE	Alfason® Repair	18I90/75	1
Karo Pharma/Noweda	Alfason® Repair	20F45/77	1
Karopharma/Noweda	Alfason® Repair	19DA8/75	1
LeoPharma A/S /Noweda	Alfason® Repair	18B26/76	1
LeoPharma A/S /Noweda	Alfason® Repair	18I88/75	1
LeoPharma A/S /Noweda	Alfason® Repair	19D05/75	1
Phoenix	Alfason® Repair	15/03/75	1
Phönix	Alfason® Repair	15J09/75	1
PHÖNIX	Alfason® Repair	17E77/75	2
PHÖNIX	Alfason® Repair	17E81/75	2
PHÖNIX	Alfason® Repair	17F72/75	1

- 15 414 spectra from 1165 *Apo-Ident* customers from a total of 5008 batches from a further 158 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 *Alfason® Repair* 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 *Alfason® Repair* 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	255	0	28 300
Type B	0	22	18	26 061
Type C	0	14	5	15 412

The substance/substance group *Alfason® Repair* 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 % (> 99.9637 %)	100.0000 % (> 97.6471 %)
Type B	100.0000 % (> 99.9514 %)	55.0000 % (> 47.5000 %)
Type C	100.0000 % (> 98.9584 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Alfason® Repair* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Alfason Basis Cresa®	10.66	–
Dermatop® base ointment	16.50	–
Excipial® lipo cream	39.24	–
ALLERGIKA®-Lipolotio urea 5% F	46.15	–
Neuroderm® moisturising cream lipo	62.25	–

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

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
30724	30724	0.00	20.26
31069	31069	0.00	9.14
32993	32993	0.00	15.61
33790	33790	0.00	16.50

continued on the next page

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continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
35476	35476	0.00	17.59
36758	36758	0.00	22.67

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 2.5-2023-04

Validated substance/substance group	**Allergika evening primrose oil cream 20% / Dermifant® kids cr**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30970-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Allergika evening primrose oil cream 20% / Dermifant® kids cream; ALLERGIKA® – Nachtkerzenöl Creme 20%; Dermifant® kids cream

Special notes

When selecting the *Allergika evening primrose oil cream 20% / Dermifant® kids cream* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Allergika evening primrose oil cream 20% / Dermifant® kids cream	7	5	10

Second-stage model

For differentiation of the substance/substance group *Allergika evening primrose oil cream 20% / Dermifant® kids cream* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Allergika evening primrose oil cream 20% / Dermifant® kids cream*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Allergika	ALLERGIKA® – Nachtkerzenöl C…	1504021	31725	60	not required
Allergika	ALLERGIKA® – Nachtkerzenöl C…	1511051	31871	60	not required
Allergika	ALLERGIKA® – Nachtkerzenöl C…	1609043	33486	40	not required
Allergika	Dermifant® kids cream	1210082	30970	80	not required
Allergika	Dermifant® kids cream	1303033	31062	40	not required
Allergika	Dermifant® kids cream	1705043	33639	40	not required
Allergika	Dermifant® kids cream	2103037	35570	50	not required

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 370 spectra of 7 reference samples from the substance/substance group *Allergika evening primrose oil cream 20% / Dermifant® kids cream*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 28 185 spectra from a total of 597 batches from further 158 substances. These spectra were recorded by *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 by *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.

- 210 spectra of 5 reference samples from the substance/substance group *Allergika evening primrose oil cream 20% / Dermifant® kids cream*.

- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Allergika	ALLERGIKA® – Nachtkerzenöl C…	1607031	32756	40
Allergika	ALLERGIKA® – Nachtkerzenöl C…	1410062	32909	40
Allergika	ALLERGIKA® – Nachtkerzenöl C…	2103051	35571	50
Allergika	Dermifant® kids cream	1607032	32754	40
Allergika	Dermifant® kids cream	1801010	34033	40

- 25 891 spectra from a total of 583 batches from further 208 substances. These spectra were recorded by *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 3 *Apo-Ident* customers from 11 batches from the substance/substance group *Allergika evening primrose oil cream 20% / Dermifant® kids cream*.

- 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
Allergika Pharma GmbH	Dermifant® kids cream	1410072	1
Allergika Pharma/Alliance	Dermifant® kids cream	1511052	1
Allergika/Gehe	Dermifant® kids cream	1502013	1
Allergika/Phönix	Dermifant® kids cream	1509042	1
Gehe	Dermifant® kids cream	1407053	1
Phönix EK:10,19 EUR …	Dermifant® kids cream	1703024	1
Phönix	Dermifant® kids cream	1312102	2
Sanacorp /100ml	Dermifant® kids cream	1711094	4
Sanacorp WE: 01.09.17 …	Dermifant® kids cream	1705043	1
Sanacorp WE: 09.11.17 1…	Dermifant® kids cream	1708063	2
WE:Phoenix 10.12.2016 …	Dermifant® kids cream	1609042	1

- 15 417 spectra from 1165 *Apo-Ident* customers from a total of 5013 batches from a further 158 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 *Allergika evening primrose oil cream 20% / Dermifant® kids cream* 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 *Allergika evening primrose oil cream 20% / Dermifant® kids cream* 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	370	0	28 185
Type B	0	210	0	25 891
Type C	0	15	1	15 417

The substance/substance group *Allergika evening primrose oil cream 20% / Dermifant® kids cream* 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 % (> 99.9636 %)	100.0000 % (> 98.3784 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 97.1429 %)
Type C	100.0000 % (> 98.9680 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Allergika evening primrose oil cream 20% / Dermifant® kids cream* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Excipial® U Lipolotio	13.49	–
Dermatest base ointment	20.40	–
Lipoderm® lotion	20.60	–
DMS® base cream high classic	21.22	–
ALLERGIKA®-Lipolotio urea 5% F	23.21	–
DMS® base cream high classic plus	24.61	–
Hans Karrer Lipocream MicroSilver	25.81	–
Abitima® clinic body cream	27.14	–
Excipial® U10 Lipolotio	36.58	–
Neuroderm® moisturising cream	39.06	–
Neuroderm® moisturising cream lipo	39.83	–
Eucerinum W/O basis	44.29	–
DMS® base cream classic	47.95	–
Base cream DVL-P	51.23	–

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

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

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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
30970	30970	0.00	17.44
31062	31062	0.00	20.77
31725	31725	0.00	19.09
31871	31871	0.00	17.80
33486	33486	0.00	18.24
33639	33639	0.00	18.56
35570	35570	0.00	16.56

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 2.5-2023-04

Validated substance/substance group	**ALLERGIKA® – Eyelid cream MED**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`10005284-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

ALLERGIKA® – Eyelid cream MED

Special notes

When selecting the *ALLERGIKA® – Eyelid cream MED* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
ALLERGIKA® – Eyelid cream MED	2	1	0

Second-stage model

For differentiation of the substance/substance group *ALLERGIKA®* – *Eyelid cream MED* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *ALLERGIKA®* – *Eyelid cream MED*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Allergika	ALLERGIKA® – Eyelid cream MED	2103030	35499	40	not required
Allergika	ALLERGIKA® – Eyelid cream MED	2007042	35501	40	not required

Validation samples

A total of 70 089 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 *ALLERGIKA®* – *Eyelid cream MED*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 28 475 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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 *ALLERGIKA®* – *Eyelid cream MED*.
- 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
Allergika	ALLERGIKA® – Eyelid cream MED	2102010	35500	40

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- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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 *ALLERGIKA® – Eyelid cream MED*.
- 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.
- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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 *ALLERGIKA® – Eyelid cream MED* 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 *ALLERGIKA® – Eyelid cream MED* 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	28 475
Type B	0	40	0	26 061
Type C	0	0	0	15 433

The substance/substance group *ALLERGIKA® – Eyelid cream MED* 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 % (> 99.9642 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9514 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *ALLERGIKA® – Eyelid cream MED* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Neuroderm® moisturising cream	7.68	–
Hans Karrer Lipocream MicroSilver	9.68	–
Abitima® clinic body cream	9.96	–
DMS® base cream high classic	10.87	–
Eucerinum W/O basis	11.34	–
DMS® base cream classic	11.56	–
Excipial® U Lipolotio	14.96	–
Base cream Taoasis	15.51	–
Base cream DVL-P	18.89	–
Excipial® U10 Lipolotio	19.19	–
DMS® base cream high classic plus	20.01	–
Linola® body milk	22.84	–
Lipoderm® lotion	23.42	–
ALLERGIKA® – Face cream MED	24.52	–
Neribas® cream	24.89	–
Asche Basis® lotion	25.62	–
Asche Basis® cream	27.99	–
Neuroderm® care lotion	28.20	–
Excipial® hydro cream	32.94	–
Dermatop® base cream	37.81	–
La Roche-Posay Toleriane	38.44	–
Fabitop® base cream	39.14	–
Dimeticone ointment 10% SR	40.81	–
ALLERGIKA®-Lipolotio urea 5% F	42.07	–
Dermatest base ointment	46.04	–
Hans Karrer Lipolotion MicroSilver	46.66	–
ALLERGIKA® – Nachtkerzenöl Creme 20%	51.87	–

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

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
35499	35499	0.00	10.65
35501	35501	0.00	13.76

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**ALLERGIKA®-Lipolotio urea 5% F**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30973-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

ALLERGIKA®-Lipolotio urea 5% F

Special notes

When selecting the *ALLERGIKA®-Lipolotio urea 5% F* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
ALLERGIKA®-Lipolotio urea 5% F	4	1	3

Second-stage model

For differentiation of the substance/substance group *ALLERGIKA®-Lipolotio urea 5% F* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *ALLERGIKA®-Lipolotio urea 5% F*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Allergika	ALLERGIKA®-Lipolotio urea 5% F	1205050	30973	80	not required
Allergika	ALLERGIKA®-Lipolotio urea 5% F	13112021	31766	60	not required
Allergika	ALLERGIKA®-Lipolotio urea 5% F	1801022	34362	40	not required
Allergika	ALLERGIKA®-Lipolotio urea 5% F	2011033	35569	50	not required

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 230 spectra of 4 reference samples from the substance/substance group *ALLERGIKA®-Lipolotio urea 5% F*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 28 325 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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 *ALLERGIKA®-Lipolotio urea 5% F*.

- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Allergika	ALLERGIKA®-Lipolotio urea 5% F	1502011	32766	40
Allergika	ALLERGIKA®-Lipolotio urea 5% F	1502011	33482	40

- 26 021 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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 3 *Apo-Ident* customers from 3 batches from the substance/substance group *ALLERGIKA®-Lipolotio urea 5% F*.
- 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
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

- 15 430 spectra from 1165 *Apo-Ident* customers from a total of 5021 batches from a further 158 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 *ALLERGIKA®-Lipolotio urea 5% F* 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 *ALLERGIKA®-Lipolotio urea 5% F* 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	230	0	28 325
Type B	0	80	0	26 021
Type C	0	3	0	15 430

The substance/substance group *ALLERGIKA®-Lipolotio urea 5% F* 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 % (> 99.9637 %)	100.0000 % (> 97.3913 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9820 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *ALLERGIKA®-Lipolotio urea 5% F* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Dermatest base ointment	15.33	–
Neuroderm® moisturising cream lipo	17.19	–
Excipial® U Lipolotio	32.53	–
ALLERGIKA® – Nachtkerzenöl Creme 20%	38.09	–
Dermifant® kids cream	49.75	–
Abitima® clinic body cream	53.22	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *ALLERGIKA®-Lipolotio urea 5% F* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

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
30973	30973	0.00	18.90
31766	31766	0.00	31.52
34362	34362	0.00	25.38
35569	35569	0.00	17.11

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**alpha-bisabolol (racemic) at least 85%**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31464-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

alpha-bisabolol (racemic) at least 85%

Special notes

When selecting the *alpha-bisabolol (racemic) at least 85%* substance/substance group, the following information is displayed to the user:

- Advice: Currently no longer available. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
alpha-bisabolol (racemic) at least 85%	1	3	9

Second-stage model

For differentiation of the substance/substance group *alpha-bisabolol (racemic) at least 85%* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *alpha-bisabolol (racemic) at least 85%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	alpha-bisabolol (racemic) at…	13360114	31464	60	not required
Caelo	alpha-bisabolol (racemic) at…	13360114	31465	60	not required

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 2 reference samples from the substance/substance group *alpha-bisabolol (racemic) at least 85%*. These samples are listed above in the *calibration samples* section. The reference samples come from 1 different batches.

- 28 435 spectra from a total of 603 batches from further 159 substances. These spectra were recorded by *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 by *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 *alpha-bisabolol (racemic) at least 85%*.

- 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	alpha-bisabolol (racemic) at…	16271902	32782	40
Caelo	alpha-bisabolol (racemic) at…	17065801	33417	40
Caelo	alpha-bisabolol (racemic) at…	180585	34227	40

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- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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 8 *Apo-Ident* customers from 9 batches from the substance/substance group *alpha-bisabolol (racemic) at least 85%*.

- 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
Caelo	alpha-bisabolol (racemic) at…	14322713	1
Caelo	alpha-bisabolol (racemic) at…	18058503	1
Caelo	alpha-bisabolol (racemic) at…	18058504	1
Caelo	alpha-bisabolol (racemic) at…	18058506	1
Caelo	alpha-bisabolol (racemic) at…	18306001	2
Caelo	alpha-bisabolol (racemic) at…	18306002	1
Caesar & Loretz GmbH	alpha-bisabolol (racemic) at…	19000485002	1
Spangro 28.01.2019	alpha-bisabolol (racemic) at…	18058506	1
Spangro 28.1.2019	alpha-bisabolol (racemic) at…	180580506	1
Spinnrad	alpha-bisabolol (racemic) at…	920303032	1

- 15 422 spectra from 1165 *Apo-Ident* customers from a total of 5015 batches from a further 158 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 *alpha-bisabolol (racemic) at least 85%* 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 *alpha-bisabolol (racemic) at least 85%* 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	28 435
Type B	0	120	0	25 981
Type C	0	11	0	15 422

The substance/substance group *alpha-bisabolol (racemic) at least 85%* 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 % (> 99.9639 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9695 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *alpha-bisabolol (racemic) at least 85%* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Citronella oil	46.93	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *alpha-bisabolol (racemic) at least 85%* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

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
31464	31464	0.00	50.44
31465	31465	0.00	50.44

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Angelica root oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30535-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	5	3	7

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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	20	not required

Validation samples

A total of 70 089 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 *Angelica root oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 28 315 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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 4 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.

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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
Taoasis	Angelica root oil	B3039-9598	35074†	20

- 25 961 spectra from a total of 584 batches from further 209 substances. These spectra were recorded by *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 7 batches from the substance/substance group *Angelica root 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
Caelo	Angelica root oil	11352706	1
Taoasis	Angelica root oil	1049239-3525	1
Taoasis	Angelica root oil	129271	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

- 15 426 spectra from 1165 *Apo-Ident* customers from a total of 5017 batches from a further 158 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	240	0	28 315
Type B	0	120	20	25 961
Type C	0	6	1	15 426

†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*.

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 % (> 99.9637 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9509 %)	85.7143 % (> 83.5714 %)
Type C	100.0000 % (> 98.9722 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Angelica root oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Dwarf pine oil	16.46	–
Frankincense oil	21.74	–
Juniper oil	21.86	–
Spearmint oil	25.49	–
Cypress oil	25.98	–
Silver fir oil	27.48	–
Marjoram oil	29.02	–
Pine silvestris oil	29.44	–
Swiss pine oil	30.36	–
Spruce needle oil	32.50	–
Citus oil	42.40	–
Cumin oil	44.99	–
Camphor oil	45.65	–
Hyssop oil	45.83	–

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.

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:

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30964	30964	0.00	28.85
31682	31682	0.00	26.01
31780	31780	0.00	29.86
32068	32068	0.00	25.67
35074	35074	0.00	16.77

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 2.5-2023-04

Validated substance/substance group	**Anise oil, organic**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30670-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	37

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 415 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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

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Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Anise oil, organic	42803-290	33875	40

- 25 901 spectra from a total of 584 batches from further 209 substances. These spectra were recorded by *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.

- 50 spectra from 25 *Apo-Ident* customers from 39 batches from the substance/substance group *Anise oil, organic*.

- Among them are spectra of independent samples from 37 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 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
Caelo	Anise oil, organic	20003664001	2
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/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
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	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	1

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Supplier	Substance	Batch	Spectra
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

- 15 383 spectra from 1163 *Apo-Ident* customers from a total of 4985 batches from a further 158 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	28 415
Type B	0	173	27	25 861
Type C	0	45	5	15 383

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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9512 %)	86.5000 % (> 85.0000 %)
Type C	100.0000 % (> 98.9658 %)	90.0000 % (> 84.0000 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Anise oil, organic* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

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Substance	Distance in main model	Distance in second-stage model
Fennel oil	44.48	–
Basil oil	83.61	–

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.

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	44.48
32794	32794	0.00	46.37
32935	32935	0.00	49.65

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 2.5-2023-04

Validated substance/substance group	**Argan oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`32168-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Argan oil; Oleum Arganiae

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Argan oil	2	2	6

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Argan oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Argan oil	161443	32168	60	-*
Caelo	Argan oil	16035101	32571	40	not required

Validation samples

A total of 70 089 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 *Argan oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 28 455 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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 *Argan 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.

*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	Argan oil	162759	32679	40
Caelo	Argan oil	190980	34461	40
Caelo	Argan oil	16035101	32306	40

- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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 *Argan 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
Argania Spinosa	Argan oil	A02148	1
Caelo	Argan oil	17198305	1
Caelo	Argan oil	18122701	1
Caelo	Argan oil	18163404	1
Caelo	Argan oil	18163408	1
Caesar & Loretz GmbH	Argan oil	18122701	1
Caesar & Loretz GmbH	Argan oil	19116406	1

- 15 426 spectra from 1165 *Apo-Ident* customers from a total of 5018 batches from a further 158 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 *Argan 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 *Argan 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	28 455
Type B	0	120	0	25 981
Type C	0	7	0	15 426

The substance/substance group *Argan 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 % (> 99.9640 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9722 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Argan oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Balm Bio Nature	10.84	–
Excipial® almond oil ointment	23.43	–
Salmon oil	48.95	–

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

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
32168	32168	0.00	18.21
32571	32571	0.00	14.63

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Balm Bio Nature**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31645-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Balm Bio Nature

Special notes

When selecting the *Balm Bio Nature* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Balm Bio Nature	3	2	0

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Balm Bio Nature*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Balm Bio Nature	150422-5106	31645	60	not required
Taoasis	Balm Bio Nature	150422-5106	31724	60	not required
Taoasis	Balm Bio Nature	151210-5337	32994	40	not required
Taoasis	Balm Bio Nature	180515-8060	34115	40	not required

Validation samples

A total of 70 089 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 *Balm Bio Nature*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

- 28 355 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Balm Bio Nature*.

- 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	Balm Bio Nature	160401-6083	32786	40
Taoasis	Balm Bio Nature	170403-7087	33436	40

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Balm Bio Nature*.

- 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.

Supplier	Substance	Batch	Spectra
Taoasis	Balm Bio Nature	151210-5337	12

- 15 421 spectra from 1165 *Apo-Ident* customers from a total of 5023 batches from a further 158 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 *Balm Bio Nature* 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 *Balm Bio Nature* 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	28 355
Type B	0	80	0	26 021
Type C	0	12	0	15 421

The substance/substance group *Balm Bio Nature* 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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9691 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Balm Bio Nature* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Excipial® almond oil ointment	9.88	–
Argan oil	14.07	–
Wax ointment (stabilised)	46.50	–
Salmon oil	47.39	–
Salicylic white paraffin 10%	56.26	–

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

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
31645	31645	0.00	15.59
31724	31724	0.00	19.28
32994	32994	0.00	9.88
34115	34115	0.00	18.79

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Banana aroma**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31105-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	16

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Banana aroma*.
- 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.

*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	Banana aroma	16089305	33496	40
Caelo	Banana aroma	20004505002	36050	40
Caelo	Banana aroma	22001475003	36738	40
Caelo	Banana aroma	16089305	33608	40

- 25 941 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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.

- 45 spectra from 29 *Apo-Ident* customers from 17 batches from the substance/substance group *Banana aroma*.

- 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
Caelo	Banana aroma	12302509	1
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	20004505001	4
Caelo	Banana aroma	20004505002	2
Caelo	Banana aroma	22001475003	1
Caesar & Loretz GmbH/Sa…	Banana aroma	19185301	1
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	22001475004	1
Phoenix	Banana aroma	20004505002	1

- 15 388 spectra from 1165 *Apo-Ident* customers from a total of 5007 batches from a further 158 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	28 415
Type B	0	160	0	25 941
Type C	0	45	0	15 388

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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 98.9660 %)	100.0000 % (> 86.6667 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Banana aroma* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Nicotine	118.82	–

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.

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:

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31105	31105	0.00	146.10
31606	31606	0.00	140.37
33687	33687	0.00	141.44

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 2.5-2023-04

Validated substance/substance group	**Basil oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30751-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Basil oil; Oleum ocimum basilicum

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	2	0

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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*:

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

Validation samples

A total of 70 089 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 *Basil oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Basil 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	Basil oil	21022-108746BAG90451	30751	40
Taoasis	Basil oil	1500312-126393	32972	40
Taoasis	Basil oil	1500312-126393	32973	40

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- 25 981 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 *Basil 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.

- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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* 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* 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	28 415
Type B	0	120	0	25 981
Type C	0	0	0	15 433

The substance/substance group *Basil 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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Basil oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, white	10.46	–
Coriander oil	14.06	–
Neroli oil	45.85	–
Matricaria oil, morrocan	51.94	–

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

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
31755	31755	0.00	161.17
33725	33725	0.00	166.82
37656	37656	0.00	14.06

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Benzoin siam oil 20%**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30456-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	1	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

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 295 spectra from a total of 598 batches from further 159 substances. These spectra were recorded by *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 by *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 *Benzoin siam oil 20%*.
- 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.

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

- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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
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
Taosis	Benzoin siam oil 20%	474084-96350	1

- 15 415 spectra from 1165 *Apo-Ident* customers from a total of 5007 batches from a further 158 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	28 295
Type B	0	79	1	26 021
Type C	0	17	1	15 415

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 % (> 99.9637 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9511 %)	98.7500 % (> 95.0000 %)
Type C	100.0000 % (> 98.9677 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Benzoin siam oil 20%* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Siam benzoin	77.79	–

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.

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	92.34
31843	31843	0.00	91.96
32974	32974	0.00	97.14
33855	33855	0.00	100.19
33944	33944	0.00	101.54
37653	37653	0.00	96.88

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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 2.5-2023-04

Validated substance/substance group	**Bepanthen® Wund- und Heilsalbe**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	31048-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bepanthen® Wund- und Heilsalbe

Special notes

When selecting the *Bepanthen® Wund- und Heilsalbe* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Bepanthen® Wund- und Heilsalbe	4	2	4

Second-stage model

For differentiation of the substance/substance group *Bepanthen® Wund- und Heilsalbe* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Bepanthen® Wund- und Heilsalbe*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Bayer	Bepanthen® Wund- und Heilsalbe	GP00LB9	31048	40	not required
Bayer	Bepanthen® Wund- und Heilsalbe	GP012SS	31758	60	not required
Bayer	Bepanthen® Wund- und Heilsalbe	GP01CTH	33613	40	not required
Bayer	Bepanthen® Wund- und Heilsalbe	GP02287	35472	40	not required

Validation samples

A total of 70 089 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 *Bepanthen® Wund- und Heilsalbe*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 28 375 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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 *Bepanthen® Wund- und Heilsalbe*.

- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Bayer	Bepanthen® Wund- und Heilsalbe	GP018T5	32720	40
Bayer	Bepanthen® Wund- und Heilsalbe	GP019ZF	32948	40

- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 *Bepanthen® Wund- und Heilsalbe*.
- 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
Bayer/Phönix	Bepanthen® Wund- und Heilsalbe	GO01XHE	1
Bayer	Bepanthen® Wund- und Heilsalbe	GP01AUE	1
Bayer	Bepanthen® Wund- und Heilsalbe	GP01R60	1
Bombastus	Bepanthen® Wund- und Heilsalbe	GP01-DR9	1

- 15 429 spectra from 1165 *Apo-Ident* customers from a total of 5020 batches from a further 158 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 *Bepanthen® Wund- und Heilsalbe* 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 *Bepanthen® Wund- und Heilsalbe* 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	28 375
Type B	0	80	0	26 021
Type C	0	4	0	15 429

The substance/substance group *Bepanthen® Wund- und Heilsalbe* 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 % (> 99.9638 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9777 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Bepanthen® Wund- und Heilsalbe* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Asche Basis® ointment	12.94	–
Neribas® ointment	19.44	–
Alfason Basis Cresa®	36.05	–

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

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
31048	31048	0.00	28.23
31758	31758	0.00	32.77
33613	33613	0.00	31.41
35472	35472	0.00	27.95

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Bergamot oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30307-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	4	2	23

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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
Taoasis	Bergamot oil	3221028-121642	31784	60	not required
Taoasis	Bergamot oil	01/22BE-16535	37657	40	not required

Validation samples

A total of 70 089 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 *Bergamot oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 28 295 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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.

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

- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 25 spectra from 22 *Apo-Ident* customers from 23 batches from the substance/substance group *Bergamot oil*.

- 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
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
Caelo	Bergamot oil	192330002	1
Caelo	Bergamot oil	192330009	1
Caelo	Bergamot oil	21000945006	1
Caelo	Bergamot oil	7962	1
Kaders	Bergamot oil	130564	1
Noweda	Bergamot oil	271858	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

- 15 408 spectra from 1164 *Apo-Ident* customers from a total of 5001 batches from a further 158 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	260	0	28 295
Type B	0	80	0	26 021
Type C	0	21	4	15 408

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 % (> 99.9637 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9669 %)	84.0000 % (> 72.0000 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Bergamot oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Chamomile (essential oil)	24.23	–
Spearmint oil	37.32	–
Grapefruit oil, organic	50.25	–

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.

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:

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31641	31641	0.00	32.63
31760	31760	0.00	30.91
31784	31784	0.00	29.37
36887	36887	0.00	39.32
37657	37657	0.00	52.38

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 2.5-2023-04

Validated substance/substance group	**Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30966-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil	20	10	123

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

Calibration samples

Only spectra which have been recorded by *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
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 70 089 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 / Rosmary oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 20 different batches.

- 27 655 spectra from a total of 584 batches from further 156 substances. These spectra were recorded by *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 by *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

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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 / Rosmary 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 (essentiel 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
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

- 25 581 spectra from a total of 576 batches from further 206 substances. These spectra were recorded by *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.

- 177 spectra from 82 *Apo-Ident* customers from 126 batches from the substance/substance group *Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil*.
- Among them are spectra of independent samples from 123 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Apothker Bauer & Cie. oHG	Rosemary oil		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

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Supplier	Substance	Batch	Spectra
Bombastus	Eucalyptus oil	21001239	2
Bombastus	Eucalyptus oil	289701	1
Bombastus	Eucalyptus oil	297737	1
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
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	Eucalyptus oil	20004134004	1
Caelo	Rosemary oil	200042109012	1
Caelo	Eucalyptus oil	20004332010	1
Caelo	Rosemary oil	22000012001	1
Caelo	Eucalyptus oil	300881	1
Caelo	Rosemary oil	306506	1
Caesar & Loretz GmbH Hi…	Eucalyptus oil	15063312	1
Caesar & Loretz GmbH Hi…	Eucalyptus oil	15400203	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
Primavera	Niaouli oil	410K26	1
Primavera	Cajeput (essentiel oil)	424A28	1
PVL	Cajeput (essentiel oil)	150712	1
TAOASIS GmbH D-32758 De…	Cajeput (essentiel oil)	1989-2818	1
Taoasis/Noweda	Niaouli oil	5091MGK10	1
Taoasis/Sanacorp	Cajeput (essentiel oil)	L201323018-113057	1
Taoasis/Taoasis	Rosemary oil	128391-ESJ05	1
Taoasis/Taoasis	Niaouli oil	1500450-5752	1
Taoasis	Eucalyptus oil	107371-6271	1
Taoasis	Cajeput (essentiel oil)	1301-121889	1
Taoasis	Cajeput (essentiel oil)	1301-32758	1
Taoasis	Eucalyptus oil	130205-111868	1

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Supplier	Substance	Batch	Spectra
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	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	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	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	2
Taoasis	Cajeput (essentiel oil)	2490-5372	2
Taoasis	Cajeput (essentiel oil)	2490-6100	1
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
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)	L201323018-113057	1

- 15 256 spectra from 1164 *Apo-Ident* customers from a total of 4898 batches from a further 155 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 / Rosmary 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 / Rosmary 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	27 655
Type B	0	520	0	25 581
Type C	0	174	3	15 256

The substance/substance group *Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary 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 % (> 99.9635 %)	100.0000 % (> 99.3333 %)
Type B	100.0000 % (> 99.9508 %)	100.0000 % (> 98.8462 %)
Type C	100.0000 % (> 98.9651 %)	98.3051 % (> 96.6102 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Cajeput oil / Eucalyptus oil / Niaouli oil / Rosmary oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Rosemary camphor oil	10.56	–
Cypress oil	24.14	–
Citus oil	25.99	–
Hyssop oil	28.46	–
Ravensara oil	28.80	–
Myrtle oil	31.77	–
Marjoram oil	36.71	–
Vetiver bourbon oil	40.80	–
Angelica root oil	44.41	–
Sage oil	45.84	–
Spruce needle oil	46.65	–

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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.

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	39.03
31136	31136	0.00	56.32
31420	31420	0.00	27.94
31548	31548	0.00	49.18
31551	31551	0.00	23.02
31691	31691	0.00	17.72
31694	31694	0.00	37.39
32173	32173	0.00	58.04
32174	32174	0.00	39.15
32903	32903	0.00	30.68
32933	32933	0.00	29.83
32970	32970	0.00	44.71
33657	33657	0.00	61.01
34104	34104	0.00	25.06
34374	34374	0.00	34.34
34380	34380	0.00	44.29
34401	34401	0.00	61.44
37658	37658	0.00	61.84
37661	37661	0.00	27.65
37788	37788	0.00	56.42

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 2.5-2023-04

Validated substance/substance group	**Camphor oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`33826-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	2	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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Camphor oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 28 475 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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.
- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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	80	0	28 475
Type B	0	40	0	26 061
Type C	0	0	0	15 433

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 % (> 99.9642 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9514 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Camphor oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Angelica root oil	23.09	–
Marjoram oil	24.95	–
Hyssop oil	25.73	–
Frankincense oil	34.57	–
Citus oil	37.98	–
Cumin oil	41.20	–
Swiss pine oil	41.76	–
Silver fir oil	43.51	–
Cypress oil	45.04	–
Pine silvestris oil	46.05	–
Rosemary oil	47.44	–
Sage oil	47.81	–
Spruce needle oil	49.52	–

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.

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	31.56
33827	33827	0.00	31.10

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Cardamom oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`33813-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 475 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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 3 batches from the substance/substance group *Cardamom 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
Primavera	Cardamom oil	291F28	1
Taoasis	Cardamom oil	12207C0-N03	1
Taoasis	Cardamom oil	13749C0-N09	2

- 15 429 spectra from 1165 *Apo-Ident* customers from a total of 5021 batches from a further 158 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	28 475
Type B	0	40	0	26 061
Type C	0	4	0	15 429

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 % (> 99.9642 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9514 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.9777 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Cardamom oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Citus oil	29.54	–
Vetiver bourbon oil	39.99	–
Matricaria oil, roman	40.94	–
Manuka oil	42.21	–
Sage oil	46.39	–
Hyssop oil	49.09	–
Cumin oil	51.94	–

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.

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	46.44
33961	33961	0.00	46.39

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Carrot seed oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31555-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Carrot seed oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 25 961 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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

- 15 430 spectra from 1165 *Apo-Ident* customers from a total of 5021 batches from a further 158 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	140	0	28 415
Type B	0	140	0	25 961
Type C	0	3	0	15 430

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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 98.9820 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Carrot seed oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	18.06	–
Tea tree oil	24.94	–
Patchouli oil	41.04	–
Matricaria oil, morrocan	48.93	–
Thyme oil, white	50.04	–

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.

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	36.40
32812	32812	0.00	60.86
34282	34282	0.00	57.05

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Cedar wood oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30654-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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

Calibration samples

Only spectra which have been recorded by *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 Bau…	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 70 089 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.
- 28 395 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 25 941 spectra from a total of 584 batches from further 209 substances. These spectra were recorded by *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/Phönix	Cedar wood oil	3292687	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

- 15 402 spectra from 1165 *Apo-Ident* customers from a total of 5003 batches from a further 158 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	28 395
Type B	0	120	40	25 941
Type C	0	31	0	15 402

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 % (> 99.9638 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9509 %)	75.0000 % (> 73.1250 %)
Type C	100.0000 % (> 98.9665 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Cedar wood oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Citus oil	16.58	–
Hyssop oil	19.66	–
Vetiver bourbon oil	21.50	–
Ginger oil	24.30	–
Marjoram oil	27.26	–
Cypress oil	28.47	–
Myrtle oil	34.79	–
Yarrow oil	35.61	–
Salmon oil	38.76	–
Rosemary oil	39.43	–
Angelica root oil	41.01	–
Cajeput (essentiel oil)	42.56	–
Immortelle oil	43.85	–
Niaouli oil	49.92	–

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.

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:

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31777	31777	0.00	67.77
31851	31851	0.00	19.66
33199	33199	0.00	65.02

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 2.5-2023-04

Validated substance/substance group	**Chamomile (essential oil)**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`33811-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	2	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

Calibration samples

Only spectra which have been recorded by *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
Taoasis	Chamomile (essential oil)	934	33825	30	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 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 190 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.

- 28 365 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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.

- 90 spectra of 3 reference samples from the substance/substance group *Chamomile (essential 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.

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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†	10

- 26 011 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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

- 15 431 spectra from 1165 *Apo-Ident* customers from a total of 5022 batches from a further 158 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	190	0	28 365
Type B	0	67	23	26 011
Type C	0	2	0	15 431

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:

†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*.

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9638 %)	100.0000 % (> 96.8421 %)
Type B	100.0000 % (> 99.9510 %)	74.4444 % (> 71.1111 %)
Type C	100.0000 % (> 98.9905 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Chamomile (essential oil)* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Bergamot oil	16.21	–
Spearmint oil	34.96	–
Citronella oil	42.13	–
Carrot seed oil	43.69	–
Marjoram oil	44.34	–
Lemon grass oil	50.41	–

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.

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	50.41
33825	33825	0.00	22.06
33952	33952	0.00	24.15
33963	33963	0.00	51.18
37683	37683	0.00	68.11

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,

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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 2.5-2023-04

Validated substance/substance group	**Cinnamon bark oil, Ceylon**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30957-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	4	1	3

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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Cinnamon bark oil, Ceylon*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 28 375 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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.

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

- 26 021 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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 3 batches from the substance/substance group *Cinnamon bark oil, Ceylon*.
- 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/06.08...	Cinnamon bark oil, Ceylon	1787-10972	1
Taoasis	Cinnamon bark oil, Ceylon	12217IN-N02	1
Taoasis	Cinnamon bark oil, Ceylon	415-129078	4

- 15 427 spectra from 1165 *Apo-Ident* customers from a total of 5021 batches from a further 158 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	180	0	28 375
Type B	0	80	0	26 021
Type C	0	6	0	15 427

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 % (> 99.9638 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9734 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Cinnamon bark oil, Ceylon* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Siam benzoin	106.65	–

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.

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	219.79
31648	31648	0.00	176.18
34107	34107	0.00	178.16
34375	34375	0.00	106.65

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Citric oil / Lime oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31544-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	71

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

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 135 spectra from a total of 596 batches from further 158 substances. These spectra were recorded by *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 by *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.

- 260 spectra of 6 reference samples from the substance/substance group *Citric oil / Lime 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.

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

- 25 841 spectra from a total of 584 batches from further 208 substances. These spectra were recorded by *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.

- 109 spectra from 82 *Apo-Ident* customers from 73 batches from the substance/substance group *Citric oil / Lime oil*.

- Among them are spectra of independent samples from 70 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Bergland	Citric oil		1
Bergland	Citric oil	K603901	1
bergland	Citric oil	K703167	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	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	17321104	2
Caelo	Citric oil	18092202	4

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Supplier	Substance	Batch	Spectra
Caelo	Citric oil	18092216	2
Caelo	Citric oil	18328003	4
Caelo	Citric oil	20004025013	1
Caelo	Citric oil	21003697003	1
Caelo	Citric oil	22001195001	1
Caelo	Citric oil	2416Q-01973	1
Caelo	Citric oil	91(18092216)	1
Caelo	Citric oil	W373	1
Casida	Citric oil	CA3A	1
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	17B14B04341736	1
Fagron	Citric oil	17B14-B04-350559	2
Fagron	Citric oil	17B14-B04-352490	1
Fagron	Citric oil	19K11-F08	1
Hänseler	Citric oil		3
Kögl	Citric oil	182006163916	1
Noweda	Citric oil	2947IT-K05	1
Primavera/ Phönix	Citric oil	595G26	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
Sanacorp	Citric oil	15182703	1
Taoasis/Sanaorp	Lime oil	867_124704I05	1
Taoasis/Taoasis	Lime oil	867-124956	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

- 15 324 spectra from 1158 *Apo-Ident* customers from a total of 4951 batches from a further 157 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

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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	28 135
Type B	0	260	0	25 841
Type C	0	109	0	15 324

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 % (> 99.9636 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9508 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 98.9653 %)	100.0000 % (> 94.4954 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Citric oil / Lime oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Mandarin oil, green	16.48	–
Grapefruit oil, organic	20.27	–
Dwarf pine oil	31.21	–
Orange oil	32.87	–
Silver fir oil	36.75	–
Marjoram oil	41.96	–
Tea tree oil	46.09	–
Cypress oil	51.00	–

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.

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	36.75
31558	31558	0.00	16.48
31838	31838	0.00	16.68
33611	33611	0.00	16.17
33874	33874	0.00	39.29
33942	33942	0.00	38.72
34393	34393	0.00	30.26
37664	37664	0.00	68.80

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Citronella oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31550-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	2	10

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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 *Citronella 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	Citronella oil	108494-126305	32798	40
Taoasis	Citronella oil	108494-126776	33047	40

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 11 *Apo-Ident* customers from 10 batches from the substance/substance group *Citronella oil*.

- 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
Apotheker Bauer und Cie…	Citronella oil	7444171705	1
Bombastus	Citronella oil	18004737	1
Bombastus	Citronella oil	19001887	1
Bombastus	Citronella oil	19003198	1
Bombastus	Citronella oil	19004993	2
Caelo	Citronella oil	19059006	1
Caelo	Citronella oil	200002042002	1
Caelo	Citronella oil	20003597002	1
Kögl	Citronella oil	228107163016	1
Taoasis	Citronella oil	5211028-120284	1

- 15 422 spectra from 1165 *Apo-Ident* customers from a total of 5014 batches from a further 158 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	28 355
Type B	0	80	0	26 021
Type C	0	11	0	15 422

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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9695 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Citronella oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Rose-geranium oil, organic	30.76	–
Palmarosa oil, organic	42.58	–
alpha-bisabolol (racemic) at least 85%	42.67	–
Patchouli oil	42.85	–
Marjoram oil	44.45	–
Tea tree oil	47.16	–
Lemon grass oil	51.60	–

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.

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	35.57
31840	31840	0.00	38.80
33728	33728	0.00	35.25
34409	34409	0.00	38.88

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Citus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrai**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30961-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil; Citus 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 *Citus 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Citus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil	24	18	92

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Citus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Citus oil	00438D25	33760	40	not required
Primavera	Citus oil	00621G26	34294	40	not required
Primavera	Citus oil	00673L26	34395	40	not required
Taoasis	Citus oil	788	33816	40	not required
Primavera	Clary sage oil	00529M26	34367	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 Bau…	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
Primavera	Myrtle oil	00401D25	33797	40	not required
Primavera	Myrtle oil	00877L25	33957	40	not required
Taoasis	Myrtle oil	013	33830	40	not required
Apotheker Bau…	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 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1100 spectra of 24 reference samples from the substance/substance group *Citus 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 24 different batches.

- 27 455 spectra from a total of 580 batches from further 154 substances. These spectra were recorded by *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.

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

- 840 spectra of 21 reference samples from the substance/substance group *Citus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil*.
- Among them are spectra of independent samples from 18 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	Citus oil	00348C26	34178	40
Taoasis	Citus oil	1510-135	33817	40
Taoasis	Citus 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
Taoasis	Lavender oil	17283-BG-R06	37654	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

- 25 261 spectra from a total of 568 batches from further 204 substances. These spectra were recorded by *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.

- 134 spectra from 69 *Apo-Ident* customers from 93 batches from the substance/substance group *Citus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil*.
- Among them are spectra of independent samples from 92 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
bergl	Lavender oil	K704066	1
Bergland	Lavender oil	K502790	1
Bergland	Lavender oil	K704088	1
Bombastus	Lavender oil	18000582	1
Bombastus	Lavender oil	19001102	2
Bombastus	Lavender oil	19004173	1
Bombastus	Lavender oil	20003765	1
Bombastus	Lavender oil	20004664	1
Bombastus	Lavender oil	21000345	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	80311204	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	18b26b02352705	1
Caelo	Lavender oil	191847007	1
Caelo	Lavender oil	191847010	1
Caelo	Lavender oil	21001627009	1
Caelo	Lavender oil	21001627014	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
Primavera/Noweda	Lavender oil	378E25	1
Primavera/Phoenix	Lavender oil	326C26	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
Taoasis/AHD	Lavender oil	13422BG-N09	1
Taoasis/Noweda	Lavender oil	16716-126380/11	1
Taoasis/Phoenix/10.02.2...	Lavender oil	5083	1
Taoasis/Taoasis	Lavender oil	L665-5037	1

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Supplier	Substance	Batch	Spectra
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	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	16082301/2016-2908	1
Taoasis	Lavender oil	16082301/2016-2909	4
Taoasis	Lavender oil	170001022016-5298	1
Taoasis	Clary sage oil	1700-125289	2
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

- 15 299 spectra from 1163 *Apo-Ident* customers from a total of 4931 batches from a further 155 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 *Citus 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 *Citus 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	1100	0	27 455
Type B	0	830	10	25 261
Type C	0	134	0	15 299

The substance/substance group *Citus 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 % (> 99.9635 %)	100.0000 % (> 99.4545 %)
Type B	100.0000 % (> 99.9508 %)	98.8095 % (> 98.4524 %)
Type C	100.0000 % (> 98.9652 %)	100.0000 % (> 95.5224 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Citus oil / Lavender oil / Clary sage oil / Myrtle oil / Petitgrain oil / Hyssop oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Ravensara oil	20.22	–
Rosemary oil	24.27	–
Neroli oil	25.06	–
Cypress oil	25.32	–
Marjoram oil	25.33	–
Thyme oil, white	26.94	–
Angelica root oil	28.91	–
Melissa oil 30%	29.00	–
Cedar wood oil	32.82	–
Sage oil	35.98	–
Vetiver bourbon oil	37.52	–
Yarrow oil	40.01	–
Rosemary camphor oil	40.11	–
Matricaria oil, morrocan	41.27	–
Bergamot oil	44.30	–
Ginger oil	45.30	–
Niaouli oil	45.43	–
Cajeput (essentiel oil)	47.74	–
Matricaria oil, roman	48.79	–
Camphor oil	48.83	–
Spearmint oil	51.68	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citus 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.

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

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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	51.64
30962	30962	0.00	63.91
31649	31649	0.00	40.85
31669	31669	0.00	53.18
31756	31756	0.00	70.42
31778	31778	0.00	74.22
31782	31782	0.00	42.19
31850	31850	0.00	43.31
31852	31852	0.00	32.73
32980	32980	0.00	20.22
33024	33024	0.00	64.69
33033	33033	0.00	54.80
33760	33760	0.00	40.80
33797	33797	0.00	34.70
33804	33804	0.00	69.28
33816	33816	0.00	32.82
33830	33830	0.00	44.83
33957	33957	0.00	33.49
34294	34294	0.00	34.30
34367	34367	0.00	83.77
34395	34395	0.00	35.66
37666	37666	0.00	53.34
37686	37686	0.00	26.60
37783	37783	0.00	50.64

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 2.5-2023-04

Validated substance/substance group	**Clove oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31270-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	1	12

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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 *Clove 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	Clove oil	1598-124689	32938	40
Taoasis	Clove oil	1598-124689	32940	40

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- 26 021 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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 12 *Apo-Ident* customers from 12 batches from the substance/substance group *Clove oil*.

- Among them are spectra of independent samples from 12 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	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
Caesar & Loretz GmbH/sa…	Clove oil	20003989004	1
Primavera/Sanacorp	Clove oil	133A25	1
Primavera	Clove oil	47G24	1

- 15 420 spectra from 1164 *Apo-Ident* customers from a total of 5012 batches from a further 158 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	28 355
Type B	0	80	0	26 021
Type C	0	12	1	15 420

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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9688 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Clove oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Siam benzoin	374.50	–

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.

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	451.66
31270	31270	0.00	451.68
31557	31557	0.00	434.18
31683	31683	0.00	441.16

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Common wormwood oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30842-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Common wormwood oil; Oleum artemisia vulgaris

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Common wormwood oil	2	2	1

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Common wormwood oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
ASAV Apotheke…	Common wormwood oil	10116310555	31637	60	not required
ASAV Apotheke…	Common wormwood oil	10409310558	34209	40	not required

Validation samples

A total of 70 089 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 *Common wormwood oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 28 455 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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 *Common wormwood 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
ASAV Apotheken-Service	Common wormwood oil	10815310556	32770	40
Taoasis	Common wormwood oil	7.9363	30842	40

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Supplier	Substance	Batch	Sample ID	Spectra
ASAV Apotheken-Service	Common wormwood oil	10815310556	33013	40
ASAV Apotheken-Service	Common wormwood oil	10815310556	33600	40
ASAV Apotheken-Service	Common wormwood oil	10815310556	33851	40

- 25 901 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Common wormwood 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
Caelo	Common wormwood oil	79363	1

- 15 432 spectra from 1165 *Apo-Ident* customers from a total of 5023 batches from a further 158 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 *Common wormwood 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 *Common wormwood 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	28 455
Type B	0	51	149	25 901
Type C	0	0	1	15 432

The substance/substance group *Common wormwood 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 % (> 99.9640 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9509 %)	25.5000 % (> 24.0000 %)
Type C	100.0000 % (> 99.0163 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Common wormwood oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Thuja oil	53.49	–

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

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
31637	31637	0.00	67.83
34209	34209	0.00	84.42

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Contramarum aroma**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	31007-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	93

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 315 spectra from a total of 598 batches from further 159 substances. These spectra were recorded by *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 by *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 *Contramarum aroma*.

- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Contramarum aroma	162671	32695	40
Caelo	Contramarum aroma	172230	33701	40
Caelo	Contramarum aroma	181067	34066	40

- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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.

- 263 spectra from 103 *Apo-Ident* customers from 95 batches from the substance/substance group *Contramarum aroma*.

- Among them are spectra of independent samples from 93 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	1
Alliance Healthcare	Contramarum aroma	17223007	1
Cael	Contramarum aroma	13141603	1
Caelo	Contramarum aroma	11378804	1
Caelo	Contramarum aroma	12051808	1
Caelo	Contramarum aroma	12201407	2
Caelo	Contramarum aroma	13141606	3
Caelo	Contramarum aroma	13141608	2
Caelo	Contramarum aroma	1315Q-03148	1
Caelo	Contramarum aroma	13411007	4
Caelo	Contramarum aroma	13411008	1
Caelo	Contramarum aroma	13411011	1
Caelo	Contramarum aroma	134111002	1
Caelo	Contramarum aroma	13815152	1
Caelo	Contramarum aroma	143200009	1
Caelo	Contramarum aroma	14320001	1
Caelo	Contramarum aroma	14320005	1
Caelo	Contramarum aroma	14320006	3
Caelo	Contramarum aroma	14320009	2
Caelo	Contramarum aroma	14320015	3
Caelo	Contramarum aroma	15113002	3
Caelo	Contramarum aroma	15113003	2
Caelo	Contramarum aroma	15113011	1
Caelo	Contramarum aroma	16083801	9
Caelo	Contramarum aroma	16083802	2
Caelo	Contramarum aroma	16083804	2
Caelo	Contramarum aroma	16083805	1
Caelo	Contramarum aroma	16083806	1
Caelo	Contramarum aroma	16267101	7
Caelo	Contramarum aroma	16267102	4
Caelo	Contramarum aroma	16267103	5
Caelo	Contramarum aroma	169267103	1
Caelo	Contramarum aroma	17223001	8
Caelo	Contramarum aroma	17223002	6
Caelo	Contramarum aroma	17223004	4

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Supplier	Substance	Batch	Spectra
Caelo	Contramarum aroma	17223005	5
Caelo	Contramarum aroma	17223007	7
Caelo	Contramarum aroma	17223008	2
Caelo	Contramarum aroma	18106701	1
Caelo	Contramarum aroma	18106702	8
Caelo	Contramarum aroma	18106703	12
Caelo	Contramarum aroma	18106705	1
Caelo	Contramarum aroma	18106706	2
Caelo	Contramarum aroma	19065401	12
Caelo	Contramarum aroma	19065403	5
Caelo	Contramarum aroma	19121701	1
Caelo	Contramarum aroma	19129001	4
Caelo	Contramarum aroma	19129002	3
Caelo	Contramarum aroma	192009401	1
Caelo	Contramarum aroma	19209401	6
Caelo	Contramarum aroma	19209402	2
Caelo	Contramarum aroma	19209403	3
Caelo	Contramarum aroma	192867003	4
Caelo	Contramarum aroma	192867004	1
Caelo	Contramarum aroma	192867005	2
Caelo	Contramarum aroma	192867006	1
Caelo	Contramarum aroma	2000061002	1
Caelo	Contramarum aroma	20000961002	5
Caelo	Contramarum aroma	20000961003	3
Caelo	Contramarum aroma	20002656001	3
Caelo	Contramarum aroma	20002656002	2
Caelo	Contramarum aroma	20002656005	1
Caelo	Contramarum aroma	20002656006	2
Caelo	Contramarum aroma	20004334002	3
Caelo	Contramarum aroma	2041515	1
Caelo	Contramarum aroma	21(17223001)	1
Caelo	Contramarum aroma	21002097001	1
Caelo	Contramarum aroma	21002097002	2
Caelo	Contramarum aroma	21002097004	1
Caelo	Contramarum aroma	21003710001	1
Caelo	Contramarum aroma	21003710003	1
Caelo	Contramarum aroma	2100371003	1
Caelo	Contramarum aroma	21051508	1
Caelo	Contramarum aroma	22(18106701)	1
Caelo	Contramarum aroma	22000814001	1
Caelo	Contramarum aroma	22000814002	2
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/ G...	Contramarum aroma	192867004	1
Caesar & Loretz GmbH/ G...	Contramarum aroma	20004334002	1
Caesar & Loretz GmbH/Gehe	Contramarum aroma	21003710001	1
Caesar & Loretz GmbH/Je...	Contramarum aroma	21002097003	1
Caesar & Loretz GmbH/No...	Contramarum aroma	19065401	1
Caesar & Loretz GmbH/No...	Contramarum aroma	20000961004	1
Caesar & Loretz GmbH/Ph...	Contramarum aroma	192867004	1
Caesar & Loretz GmbH	Contramarum aroma	19065401	3

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Supplier	Substance	Batch	Spectra
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	192867006	1
Caesar & Loretz GmbH	Contramarum aroma	20000961004	1
Caesar & Loretz GmbH	Contramarum aroma	20000961005	1
Caesar & Loretz GmbH	Contramarum aroma	20002656002	1
Caesar & Loretz GmbH	Contramarum aroma	21002097002	3
Caesar & Loretz GmbH	Contramarum aroma	21003710001	1
Caesar & Loretz GmbH	Contramarum aroma	22000814004	2
Caesar & Loretz GmbH	Contramarum aroma	22002935001	1
Caesar & Loretz GmbH	Contramarum aroma	22002935002	3
Fagron	Contramarum aroma	16083801	1
Fiebig	Contramarum aroma	11378810	1
Gehe	Contramarum aroma	12201404	1
Gehe	Contramarum aroma	20000961002	1
Phoenix Goettin	Contramarum aroma	70401432001	1
Phönix	Contramarum aroma	17223007	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

- 15 170 spectra from 1154 *Apo-Ident* customers from a total of 4929 batches from a further 158 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	28 315
Type B	0	120	0	25 981
Type C	0	262	1	15 170

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 % (> 99.9637 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9650 %)	99.6198 % (> 98.4791 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Contramarum aroma* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Raspberry aroma	39.77	–
Strawberry aroma	79.75	–

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.

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	60.20
31289	31289	0.00	55.96
31398	31398	0.00	58.66
35897	35897	0.00	58.74
36582	36582	0.00	58.09
37456	37456	0.00	61.20

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Cumin oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30449-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	2	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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Cumin oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 28 435 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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/Noweda	Cumin oil	51764-124373BAG9045	1
Taoasis	Cumin oil	104723-298	1
Taoasis	Cumin oil	121217-111221	1
Taoasis	Cumin oil	24081-106027	1

- 15 429 spectra from 1165 *Apo-Ident* customers from a total of 5020 batches from a further 158 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	120	0	28 435
Type B	0	120	0	25 981
Type C	0	3	1	15 429

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 % (> 99.9639 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9777 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Cumin oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	96.34	–

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.

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	139.64
32267	32267	0.00	137.08
32904	32904	0.00	142.28

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Cypress oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30457-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	15

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 335 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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.

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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

- 25 941 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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.

- 25 spectra from 3 *Apo-Ident* customers from 16 batches from the substance/substance group *Cypress 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
Primavera	Cypress oil	431C27	1
Taoasis	Cypress oil	1039-121894	3
Taoasis	Cypress oil	1039-122434	1
Taoasis	Cypress oil	107527-125443	2
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

- 15 408 spectra from 1165 *Apo-Ident* customers from a total of 5008 batches from a further 158 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	28 335
Type B	0	155	5	25 941
Type C	0	25	0	15 408

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 % (> 99.9637 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9509 %)	96.8750 % (> 95.0000 %)
Type C	100.0000 % (> 98.9669 %)	100.0000 % (> 76.0000 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Cypress oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	22.76	–
Citus oil	30.24	–
Myrtle oil	33.70	–
Dwarf pine oil	40.47	–
Ginger oil	46.74	–
Spearmint oil	50.20	–

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.

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	69.80
33623	33623	0.00	67.49
33802	33802	0.00	48.10

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33954	33954	0.00	48.72
37678	37678	0.00	69.97

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 2.5-2023-04

Validated substance/substance group	**Dermatop® base ointment**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	31060-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dermatop® base ointment

Special notes

When selecting the *Dermatop® base ointment* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Dermatop® base ointment	3	2	59

Second-stage model

For differentiation of the substance/substance group *Dermatop® base ointment* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Dermatop® base ointment*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Sanofi aventis	Dermatop® base ointment	3F052A	31060	40	not required
Sanofi aventis	Dermatop® base ointment	5F080A	31717	60	not required
Sanofi aventis	Dermatop® base ointment	1F151A	36038	40	not required

Validation samples

A total of 70 089 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 *Dermatop® base ointment*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Dermatop® base ointment*.
- 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
Sanofi aventis	Dermatop® base ointment	5F089A	32718	40
Sanofi aventis	Dermatop® base ointment	7F106A	33965	40

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 196 spectra from 33 *Apo-Ident* customers from 60 batches from the substance/substance group *Dermatop® base ointment*.

- Among them are spectra of independent samples from 59 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	Dermatop® base ointment	5F080A	1
Caelo	Dermatop® base ointment	7F107A	1
Caelo	Dermatop® base ointment	8F124A	1
Caelo	Dermatop® base ointment	8F125A	2
Galderma/Noweda	Dermatop® base ointment	8F123A	2
Noweda/Sanofi	Dermatop® base ointment	F140A	2
Phönix/ Sanofi/ 02.10.2...	Dermatop® base ointment	F136A	1
Phönix	Dermatop® base ointment	7F108B	1
Sanacorp/ Sanofi	Dermatop® base ointment	9F128A	1
Sanacorp/Sanofi WE:22.0...	Dermatop® base ointment	5F086A	1
Sanofi - Noweda	Dermatop® base ointment	5F089A	1
Sanofi / Alliance Healt...	Dermatop® base ointment	6F094A	1
Sanofi / Alliance Healt...	Dermatop® base ointment	8F118A	1
Sanofi / Gehe	Dermatop® base ointment	6F099A	1
Sanofi / Gehe	Dermatop® base ointment	8F120A	1
Sanofi / Gehe	Dermatop® base ointment	8F124A	1
Sanofi / Phönix	Dermatop® base ointment	F136A	1
Sanofi / Sanacorp	Dermatop® base ointment	8F125A	1
Sanofi /Noweda	Dermatop® base ointment	1F145A	1
Sanofi /Noweda	Dermatop® base ointment	8F121A	1
Sanofi /Noweda	Dermatop® base ointment	F140A	1
Sanofi /Noweda	Dermatop® base ointment	F142A	1
Sanofi /Noweda	Dermatop® base ointment	F143A	1
Sanofi /Noweda	Dermatop® base ointment	OF135A	1
Sanofi /Noweda	Dermatop® base ointment	OF137A	1
Sanofi Aventis / Sanacop	Dermatop® base ointment	F141A	1
Sanofi Aventis/Sanacorp	Dermatop® base ointment	9F134A	1
Sanofi Aventis	Dermatop® base ointment	8F123B	2
Sanofi/ Noweda/ 09.04.2...	Dermatop® base ointment	F140A	1
Sanofi/Alliance	Dermatop® base ointment	8F119A	1
Sanofi/Gehe	Dermatop® base ointment	5F078A	1
Sanofi/GEHE	Dermatop® base ointment	8F115A	1
Sanofi/GEHE	Dermatop® base ointment	8F116A	1
Sanofi/GEHE	Dermatop® base ointment	8F117A	1
Sanofi/GEHE	Dermatop® base ointment	8F126A	1
Sanofi/Kehr	Dermatop® base ointment	6F094A	1
Sanofi/Kehr	Dermatop® base ointment	6F099A	1
Sanofi/Kehr	Dermatop® base ointment	9F133A	1
Sanofi/Kehr	Dermatop® base ointment	F136A	1
Sanofi/Kehr	Dermatop® base ointment	F143A	1
Sanofi/Noweda	Dermatop® base ointment	1F145A	1

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Supplier	Substance	Batch	Spectra
Sanofi/Noweda	Dermatop® base ointment	1F146A	5
Sanofi/Noweda	Dermatop® base ointment	1F147A	1
Sanofi/Noweda	Dermatop® base ointment	8F121A	1
Sanofi/Noweda	Dermatop® base ointment	8F123B	1
Sanofi/Noweda	Dermatop® base ointment	8F125A	1
Sanofi/Noweda	Dermatop® base ointment	8F126A	2
Sanofi/Noweda	Dermatop® base ointment	9F128A	1
Sanofi/Noweda	Dermatop® base ointment	9F129A	1
Sanofi/Noweda	Dermatop® base ointment	9F131A	1
Sanofi/Noweda	Dermatop® base ointment	9F132A	1
Sanofi/Noweda	Dermatop® base ointment	F138A	4
Sanofi/Noweda	Dermatop® base ointment	OF135A	2
Sanofi/Noweda	Dermatop® base ointment	OF138A	23
Sanofi/Noweda	Dermatop® base ointment	OF142A	3
Sanofi/Noweda	Dermatop® base ointment	OF143A	31
Sanofi/Noweda	Dermatop® base ointment	OF144A	4
Sanofi/Phoenix	Dermatop® base ointment	8F120A	1
Sanofi/Phönix	Dermatop® base ointment	7F105A	1
Sanofi/Phönix	Dermatop® base ointment	7F109A	2
Sanofi/Phönix	Dermatop® base ointment	8F113A	1
Sanofi/Phönix	Dermatop® base ointment	8F114A	1
Sanofi/Phönix	Dermatop® base ointment	8F116A	1
Sanofi/Phönix	Dermatop® base ointment	8F118B	2
Sanofi/Phönix	Dermatop® base ointment	8F119A	2
Sanofi/Phönix	Dermatop® base ointment	8F121A	3
Sanofi/Phönix	Dermatop® base ointment	8F1238	1
Sanofi/Phönix	Dermatop® base ointment	8F125A	2
Sanofi/Phönix	Dermatop® base ointment	8F126A	1
Sanofi/Phönix	Dermatop® base ointment	9F127A	1
Sanofi/Phönix	Dermatop® base ointment	9F131A	1
Sanofi/Phönix	Dermatop® base ointment	9F134A	1
Sanofi/Phönix	Dermatop® base ointment	F137A	1
Sanofi/Phönix	Dermatop® base ointment	F139A	1
Sanofi/Phönix	Dermatop® base ointment	F140A	1
Sanofi/Sanacorp	Dermatop® base ointment	8F126A	2
sanofi/Sanacorp	Dermatop® base ointment	9F128A	2
Sanofi/Sanacorp	Dermatop® base ointment	9F130A	1
Sanofi/Sanacorp	Dermatop® base ointment	9F133A	3
Sanofi/Sanacorp	Dermatop® base ointment	9F134A	4
sanofi/Sanacorp	Dermatop® base ointment	F135A	1
Sanofi/Sanacorp	Dermatop® base ointment	F137A	1
Sanofi/Sanacorp	Dermatop® base ointment	F139A	3
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	8F116A	1
sanofi	Dermatop® base ointment	8F119A	1
Sanofi	Dermatop® base ointment	8F124A	3
sanofi	Dermatop® base ointment	8F126A	1
Sanofi	Dermatop® base ointment	8F127A	1
Sanofi	Dermatop® base ointment	9F127A	1
Sanofi	Dermatop® base ointment	9F128A	1
Sanofi	Dermatop® base ointment	9F129A	3
Sanofi	Dermatop® base ointment	9F130A	1
Sanofi	Dermatop® base ointment	9F131A	1
Sanofi	Dermatop® base ointment	9F134A	2
Sanofi	Dermatop® base ointment	9F178A	1
Sanofi	Dermatop® base ointment	F138A	1
sanofi	Dermatop® base ointment	F140A	1

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Supplier	Substance	Batch	Spectra
Sanofi	Dermatop® base ointment	F142A	1
sanofi	Dermatop® base ointment	OF144A	1
Sanofi-Aventis Deutschl...	Dermatop® base ointment	9F183A	1
Sanofi-Aventis	Dermatop® base ointment	7F103A	1
Sanofi-Aventis	Dermatop® base ointment	8F117A	1

- 15 237 spectra from 1165 *Apo-Ident* customers from a total of 4964 batches from a further 158 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 *Dermatop® base 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 *Dermatop® base 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	140	0	28 415
Type B	0	80	0	26 021
Type C	0	192	4	15 237

The substance/substance group *Dermatop® base 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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9651 %)	97.9592 % (> 96.4286 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Dermatop® base ointment* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Excipial® lipo cream	19.83	–
Alfason Basis Cresa®	28.86	–
ALLERGIKA®-Lipolotio urea 5% F	35.70	–
Alfason® Repair	37.41	–
Dermatest base ointment	50.59	–

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

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
31060	31060	0.00	20.63
31717	31717	0.00	25.22
36038	36038	0.00	21.98

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Dexeryl®**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31512-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dexeryl®

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Dexeryl®	4	2	17

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Dexeryl®*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Pierre Fabre	Dexeryl®	G99016	31512	60	not required
Pierre Fabre	Dexeryl®	G00419	31630	60	not required
Pierre Fabre	Dexeryl®	G00650	33635	40	not required
Pierre Fabre	Dexeryl®	G00748	36771	40	not required

Validation samples

A total of 70 089 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 *Dexeryl®*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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 *Dexeryl®*.

- 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
Pierre Fabre	Dexeryl®	G00623	32762	40
Pierre Fabre	Dexeryl®	G00658	33945	40

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 22 spectra from 6 *Apo-Ident* customers from 18 batches from the substance/substance group *Dexeryl®*.

- 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
Noweda	Dexeryl®	G00909	1
P.Fabre/Phoenix	Dexeryl®	G00951	1
PiereFabre/Now	Dexeryl®	G00577	1
Pierre Fabre / phoenix	Dexeryl®	600869	1
Pierre Fabre /Noweda	Dexeryl®	Goo606	1
Pierre Fabre/Now	Dexeryl®	G00650	1
Pierre Fabre/Sanacorp	Dexeryl®	G00064_A	1
Pierre Fabre/Sanacorp	Dexeryl®	G00729	2
PierreFabre/ Phoenix	Dexeryl®	G00835	1
PierreFabre/ Phoenix	Dexeryl®	G00904	1
PierreFabre/ Phoenix	Dexeryl®	G00956/2x500g	1
PierreFabre/ Phoenix	Dexeryl®	G00966	2
PierreFabre/ Phoenix	Dexeryl®	G00967	2
PierreFabre/ Phoenix	Dexeryl®	G01021	2
PierreFabre/ Phoenix	Dexeryl®	G01088	1
PierreFabre/ Phoenix	Dexeryl®	G01117	1
PierreFabre/ Phoenix	Dexeryl®	G01118	1
PierreFabre/ Phoenix	Dexeryl®	G01122	1

- 15 411 spectra from 1164 *Apo-Ident* customers from a total of 5006 batches from a further 158 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 *Dexeryl®* 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 *Dexeryl®* 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	28 355
Type B	0	80	0	26 021
Type C	0	22	0	15 411

The substance/substance group *Dexeryl*® 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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9672 %)	100.0000 % (> 72.7273 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Dexeryl*® in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Neuroderm® moisturising cream	17.04	–
Neuroderm® care lotion	17.56	–
Hans Karrer Lipocream MicroSilver	18.47	–
Base cream Taoasis	20.42	–
Excipial® U10 Lipolotio	21.35	–
DMS® base cream high classic	26.18	–
Hans Karrer Lipolotion MicroSilver	26.27	–
Eucerinum O/W basis	30.03	–
DMS® base cream classic	30.32	–
Dimeticone ointment 10% SR	30.73	–
Abitima® clinic body cream	31.37	–
Dermatop® base cream	32.19	–
DMS® base cream high classic plus	35.44	–
Neribas® cream	36.19	–
Fabitop® base cream	36.68	–
La Roche-Posay Toleriane	37.49	–
Abitima® clinic face cream	37.74	–
Linola® body milk	39.05	–
Asche Basis® lotion	39.83	–
Excipial® U Lipolotio	41.90	–
Eucerinum W/O basis	46.22	–
ALLERGIKA® – Eyelid cream MED	49.57	–
Asche Basis® cream	50.78	–

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

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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
31512	31512	0.00	20.75
31630	31630	0.00	28.42
33635	33635	0.00	24.84
36771	36771	0.00	25.26

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 2.5-2023-04

Validated substance/substance group	**Dichloroacetic acid**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`10005427-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dichloroacetic acid; Acidum dichloraceticum

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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

Calibration samples

Only spectra which have been recorded by *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	S6674841614	32750	40	not required
Merck	Dichloroacetic acid	S7209041737	33794	40	not required

Validation samples

A total of 70 089 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.
- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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	S7209241824	34185	40

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- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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.
- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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	28 415
Type B	0	10	30	26 061
Type C	0	0	0	15 433

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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9514 %)	25.0000 % (> 17.5000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Dichloroacetic acid* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Nicotine	175.44	–

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.

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	229.95
32750	32750	0.00	225.62
33794	33794	0.00	245.83

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Dimeticone ointment 10% SR**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31243-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	32

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

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 425 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Dimeticone ointment 10% SR*.

- 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
apomix	Dimeticone ointment 10% SR	10A021117	33870	40
apomix	Dimeticone ointment 10% SR	02A150322	36234	40
apomix	Dimeticone ointment 10% SR	01A010223	36905	40

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- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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 11 *Apo-Ident* customers from 34 batches from the substance/substance group *Dimeticone ointment 10% SR*.

- 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
apomix	Dimeticone ointment 10% SR	10A181214	1
apomix	Dimeticone ointment 10% SR	11a271216	1
apomix	Dimeticone ointment 10% SR	11B031117	1
apomix	Dimeticone ointment 10% SR	1A070121	2
apomix	Dimeticone ointment 10% SR	1A070217	1
apomix	Dimeticone ointment 10% SR	1A120116	1
apomix	Dimeticone ointment 10% SR	1A150115	1
apomix	Dimeticone ointment 10% SR	1A150119	2
apomix	Dimeticone ointment 10% SR	1B140120	1
apomix	Dimeticone ointment 10% SR	2A180220	2
apomix	Dimeticone ointment 10% SR	2A260219	1
apomix	Dimeticone ointment 10% SR	2B150317	1
apomix	Dimeticone ointment 10% SR	3A220316	1
apomix	Dimeticone ointment 10% SR	3B040320	1
apomix	Dimeticone ointment 10% SR	3B180214	1
apomix	Dimeticone ointment 10% SR	4A010415	1
apomix	Dimeticone ointment 10% SR	4A080414	1
apomix	Dimeticone ointment 10% SR	4A230519	2
apomix	Dimeticone ointment 10% SR	4C110521	1
apomix	Dimeticone ointment 10% SR	5A020616	1
apomix	Dimeticone ointment 10% SR	5A130520	1
apomix	Dimeticone ointment 10% SR	5A200619	2
apomix	Dimeticone ointment 10% SR	5A210618	3
apomix	Dimeticone ointment 10% SR	6A190614	1
apomix	Dimeticone ointment 10% SR	6A300616	1
apomix	Dimeticone ointment 10% SR	7A151019	1
apomix	Dimeticone ointment 10% SR	7A170816	1
apomix	Dimeticone ointment 10% SR	7A310718	1
apomix	Dimeticone ointment 10% SR	7C190820	1
apomix	Dimeticone ointment 10% SR	8A041213	1
apomix	Dimeticone ointment 10% SR	8A090915	1
apomix	Dimeticone ointment 10% SR	9A051218	1
apomix	Dimeticone ointment 10% SR	9B041017	1
Euro OTC	Dimeticone ointment 10% SR	3B180214	2
PKH Halle	Dimeticone ointment 10% SR	1A310118	1

- 15 390 spectra from 1162 *Apo-Ident* customers from a total of 4990 batches from a further 158 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	28 425
Type B	0	120	0	25 790
Type C	0	43	0	15 390

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 % (> 99.9639 %)	100.0000 % (> 95.3846 %)
Type B	100.0000 % (> 99.9508 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9660 %)	100.0000 % (> 86.0465 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Dimeticone ointment 10% SR* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Hans Karrer Lipolotion MicroSilver	15.34	–
Asche Basis® lotion	18.97	–
Eucerinum W/O basis	22.62	–
DMS® base cream classic	26.80	–
Base cream Taoasis	26.82	–
La Roche-Posay Toleriane	27.04	–
DMS® base cream high classic	28.30	–
Hans Karrer Lipocream MicroSilver	29.82	–
Excipial® U Lipolotio	30.81	–
Dexeryl®	31.18	–
Neribas® cream	31.74	–
Excipial® U10 Lipolotio	31.89	–
Abitima® clinic body cream	34.97	–
Eucerinum O/W basis	36.85	–
Abitima® clinic face cream	39.14	–

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Substanz	Distance in main model	Distance in second-stage model
Linola® body milk	40.31	–
Fabitop® base cream	41.31	–
Neuroderm® moisturising cream	41.65	–
Asche Basis® cream	43.29	–
Neuroderm® care lotion	46.36	–
DMS® base cream high classic plus	50.10	–

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.

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	20.19
31638	31638	0.00	20.42
33041	33041	0.00	20.39

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 2.5-2023-04

Validated substance/substance group	**Dwarf pine oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31542-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 315 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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.

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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

- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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/Taoasis	Dwarf pine oil	25599120877	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

- 15 420 spectra from 1165 *Apo-Ident* customers from a total of 5016 batches from a further 158 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	28 315
Type B	0	120	0	25 981
Type C	0	13	0	15 420

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 % (> 99.9637 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9688 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Dwarf pine oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Cypress oil	15.12	–
Spruce needle oil	15.64	–
Pine silvestris oil	16.21	–
Silver fir oil	17.20	–
Juniper oil	19.91	–
Spearmint oil	20.95	–
Angelica root oil	21.03	–
Frankincense oil	23.47	–
Swiss pine oil	32.46	–
Marjoram oil	42.56	–
Ginger oil	44.07	–
Citus oil	49.25	–
Citric oil	52.38	–

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.

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	16.26
31689	31689	0.00	15.64
32937	32937	0.00	21.03
34109	34109	0.00	28.00
37682	37682	0.00	32.46

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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 2.5-2023-04

Validated substance/substance group	**Ethanol 70%**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30779-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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%	4	4	553

Second-stage model

For differentiation of the substance/substance group *Ethanol 70%* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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
Hofmann's	Ethanol 70%	271012	30779	80	1402563
Kremer GmbH &...	Ethanol 70%	171211	34101	40	not required

Validation samples

A total of 70 089 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 *Ethanol 70%*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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

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Supplier	Substance	Batch	Sample ID	Spectra
apomix	Ethanol 70%	09A280322	36245	40
Hofmann's	Ethanol 70%	570916	32591	40
Hofmann's	Ethanol 70%	750718	34317	40

- 25 941 spectra from a total of 584 batches from further 209 substances. These spectra were recorded by *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.

- 751 spectra from 224 *Apo-Ident* customers from 564 batches from the substance/substance group *Ethanol 70%*.

- Among them are spectra of independent samples from 550 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
— (Retest)	Ethanol 70%	181009	1
	Ethanol 70%		1
	Ethanol 70%	7023031	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/ 02...	Ethanol 70%	191121	2
A.Pflüger GmbH & Co.KG/...	Ethanol 70%	130514	1
A.Pflüger GmbH & Co.KG/...	Ethanol 70%	131011	1
A.Pflüger GmbH	Ethanol 70%	150730	1
A.Pflüger/Noweda	Ethanol 70%	130116	1
A.Pflüger	Ethanol 70%	21111301	1
AHD	Ethanol 70%	170906	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
Alte Apo Defektur	Ethanol 70%	1220E-02320	1
Alte Apo Defektur	Ethanol 70%	3019M-02320	1
Anzag/ Otto Fischar Gmb...	Ethanol 70%	7024051	1
Anzag	Ethanol 70%	7027102	1
Anzag	Ethanol 70%	7028041	3
apomix	Ethanol 70%	10A110522	2
apomix	Ethanol 70%	11A300320	1
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

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Supplier	Substance	Batch	Spectra
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 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%	2721A-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	3120Q-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	4619A-02320	3
Apotheke Hornbach Zentrum	Ethanol 70%	5219Q-02320	1
Apotheke Hornbach Zentrum	Ethanol 70%	5320I-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
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/Bahnhof...	Ethanol 70%	3819A-03043	1
Bahnhofapotheke	Ethanol 70%	130320/6/20	1
BBA	Ethanol 70%	4422E-02320	1
Behlen/Phönix	Ethanol 70%	1410T1300816	1
Belous	Ethanol 70%	4613E-02320	1
Berkel AHK/HWA	Ethanol 70%	1410T31040613/70	1
Berkel AHK	Ethanol 70%		1
Berkel AHK	Ethanol 70%	20042012397	1
Berliner Bär Apotheke	Ethanol 70%	2622I-02320	1
Berliner Bär Apotheke	Ethanol 70%	4321M-02320	1
Bombastus	Ethanol 70%	150630	1
Brennerei Gauß	Ethanol 70%		1
Brennerei Gauß	Ethanol 70%	MLOG103/20	1
Brennerei Gauß	Ethanol 70%	MLOG505/2020	1
Brennerei Gauß	Ethanol 70%	MLOG604/2020	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%	151008	2
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

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Supplier	Substance	Batch	Spectra
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 Ic...	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%	622E-03043	1
Defektur Apotheke	Ethanol 70%	819I-03043	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
Defektur/Wolf-Apotheke	Ethanol 70%	70227/52Dre	1
Defektur	Ethanol 70%		2
Defektur	Ethanol 70%	1007210429	1
Defektur	Ethanol 70%	1020211104	1
Defektur	Ethanol 70%	1026211207	1
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%	200114EtOH70	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%	270613EtOH	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

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Supplier	Substance	Batch	Spectra
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%	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%	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
Die LindenApotheke / Bl...	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/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
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

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Supplier	Substance	Batch	Spectra
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
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
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 Löwen ...	Ethanol 70%	1521E-02320	1
Eigenherstellung Löwen ...	Ethanol 70%	5220E-02320	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%	2124	1
Eigenherstellung	Ethanol 70%	2216A-02320	1
Eigenherstellung	Ethanol 70%	2314I-02320	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

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Supplier	Substance	Batch	Spectra
Eigenherstellung	Ethanol 70%	42151-02320	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
Eigenherstellung-Biozid	Ethanol 70%	FP200430-04	1
Eigenproduktion	Ethanol 70%	1217Q-02320	1
Eigenproduktion	Ethanol 70%	714Q-02320	1
Engel/Engel	Ethanol 70%	39-28715	1
Engel-Apotheke	Ethanol 70%	2319A-07016	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
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 Hea…	Ethanol 70%	7026051	1
Fischar / Alliance Hea…	Ethanol 70%	7028102	1
Fischar / Alliance Hea…	Ethanol 70%	7029041	1
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/ Phoenix/ 25.07…	Ethanol 70%	7028121	1
Fischar/ Phoenix/ 29.08…	Ethanol 70%	7029031	1
Fischar/ Sanacorp	Ethanol 70%	7021081	1
Fischar/Novatis	Ethanol 70%	701004810049	1
Fischar/Novatis	Ethanol 70%	7020113	1
Fischar/Noweda	Ethanol 70%	702004b	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
Fischar	Ethanol 70%		1
Fischar	Ethanol 70%	27031501	1
fischar	Ethanol 70%	7020012	1
Fischar	Ethanol 70%	7020046	1
Fischar	Ethanol 70%	7022022	1

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Supplier	Substance	Batch	Spectra
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	2
Fischar	Ethanol 70%	7029101	1
Fischer/Noweda	Ethanol 70%	702003F	1
Fischer/sanacorp	Ethanol 70%	702003G	1
Fischer	Ethanol 70%	7028111	1
FischerGehe	Ethanol 70%	702003H	1
fishar	Ethanol 70%	7028111	1
frischhergestellt	Ethanol 70%		2
Gehe 27.2.14	Ethanol 70%	140121	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
GEHE	Ethanol 70%	180828	1
Gehe	Ethanol 70%	3818Q-02320	1
Gehe-Kremer	Ethanol 70%	140307	1
Gehe-Kremer	Ethanol 70%	150209	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
Hermes	Ethanol 70%	3720I	1
Hetterich - Teofarma sr...	Ethanol 70%	145501/R	2
Hetterich - Teofarma sr...	Ethanol 70%	145601	3
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/AHCA	Ethanol 70%	145703	2
Hetterich/Ebert	Ethanol 70%	145401	2
Hirsch	Ethanol 70%	4413I-02320	1
Hirsch	Ethanol 70%	714E-02320	1
HirschApotheke	Ethanol 70%	10151-02320	1
HirschApotheke	Ethanol 70%	2315I-02320	1
HirschApotheke	Ethanol 70%	4614A-02320	1
Hoffmann & Sommer GmbH ...	Ethanol 70%	580916	1
Hoffmann & Sommer GmbH ...	Ethanol 70%	650917	1
Hoffmann & Sommer	Ethanol 70%	750718	1
Hoffmann / Bahnhof Apot...	Ethanol 70%	3919A-02320	1
Hoffmann	Ethanol 70%	781218	1
Hoffmanns/Anzag	Ethanol 70%	520116	1
Hofman und Sommer GmbH ...	Ethanol 70%	580916	1
Hofmann & Sommer	Ethanol 70%	691217	1
Hofmann / Phönix	Ethanol 70%	840819	1
Hofmann /Phoenix	Ethanol 70%	900320	1

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Supplier	Substance	Batch	Spectra
Hofmann et Sommer	Ethanol 70%	1000520	1
Hofmann u. Sommer	Ethanol 70%	720318	1
Hofmann und Sommer	Ethanol 70%	980520	1
Hofmanns / Noweda	Ethanol 70%	820419	1
Hofmann&Sommer GmbH und...	Ethanol 70%	940420	7
Hofmann&Sommer GmbH und...	Ethanol 70%	950420	9
Hofmann&Sommer GmbH und...	Ethanol 70%	1010520	2
Hofmann&Sommer/Sanacorp	Ethanol 70%	781218	1
Hofmann&Sommer	Ethanol 70%	940420	1
Hofmann	Ethanol 70%	320713	1
Hofmanns/AHD	Ethanol 70%	1010520	1
hofmanns/noweda	Ethanol 70%	890320	1
hofmanns/noweda	Ethanol 70%	960420	1
Hofmann's	Ethanol 70%	940420	1
Hohe-Wart-Apotheke	Ethanol 70%	23072013/1	1
Homöopathisches Laborat...	Ethanol 70%	200327	1
Hubertus Apotheke	Ethanol 70%	261113	1
Kastner (eigen)	Ethanol 70%	1215E-02320	1
Kastner (eigen)	Ethanol 70%	3114E-03043	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 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 / Noweda	Ethanol 70%	140627	1
Kremer Gmbh / Noweda	Ethanol 70%	141127	2
Kremer GmbH Wuppertal/G...	Ethanol 70%	130729	1
Kremer GmbH/Noweda	Ethanol 70%	181115	1
Kremer GmbH/Phönix	Ethanol 70%	150327	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/Alliance Healthc...	Ethanol 70%	171025	1
Kremer/Gehe	Ethanol 70%	130116	1
Kremer/Gehe	Ethanol 70%	140121	1
Kremer/Gehe	Ethanol 70%	160414	2
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
Kremer	Ethanol 70%	130206	1
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

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Supplier	Substance	Batch	Spectra
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
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 Defek...	Ethanol 70%	E-090520-1D	1
Martinus-Apotheke Defek...	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/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
Noweda	Ethanol 70%	120420	1
Noweda	Ethanol 70%	145703	1
Noweda	Ethanol 70%	145804	1
Noweda	Ethanol 70%	190717	4
Noweda	Ethanol 70%	190815	2
Noweda	Ethanol 70%	200330	1
O:Fischar/Phönix	Ethanol 70%	7027032	1
Otto Fischar GmbH & Co....	Ethanol 70%	7024021	1
Otto Fischar GmbH & Co....	Ethanol 70%	7025031	2
Otto Fischar GmbH & Co....	Ethanol 70%	7028041	1
Otto Fischar GmbH & Co....	Ethanol 70%	7024071	1
Otto Fischar GmbH & Co....	Ethanol 70%	702003D	1
Otto Fischar GmbH &Co KG	Ethanol 70%	7020043	1
Otto Fischar GmbH/ Amzag	Ethanol 70%	7024091	1
Otto Fischar GmbH/ Noweda	Ethanol 70%	7021092	1
Otto Fischar GmbH	Ethanol 70%	702003N	1
Otto Fischar/ Anzag	Ethanol 70%	7029021	1

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Supplier	Substance	Batch	Spectra
Otto Fischar	Ethanol 70%	7023111	1
Otto Fischar	Ethanol 70%	7028121	1
Otto Fischer / Noweda	Ethanol 70%	7025031	1
Otto Fischer /Phönix	Ethanol 70%	702004B	1
Otto Fischer GmbH & Co....	Ethanol 70%	7029121	1
Otto Fischer GmbH&Co.KG...	Ethanol 70%	7028091	1
Otto Fischer GmbH/Sanac...	Ethanol 70%	7021092	1
Otto Fischer GmbH	Ethanol 70%	7020031	1
Otto Fischer GmbH	Ethanol 70%	7020045	2
Otto Fischer/ Noweda	Ethanol 70%	7029051	1
otto Fischer/Noweda	Ethanol 70%	7024121	1
Otto/Fischer	Ethanol 70%	1029051	1
Pflüger 13.03.2020 EK 3...	Ethanol 70%	200303	1
Pflüger GmbH & Co.KG	Ethanol 70%	170116	1
Pflüger GmbH / Gehe	Ethanol 70%	180404	1
Pflüger GmbH / Noweda	Ethanol 70%	190717	1
Pflüger GmbH / Noweda	Ethanol 70%	200319	1
Pflüger GmbH	Ethanol 70%	191121	2
Pflüger/ Noweda	Ethanol 70%	180404	1
Pflüger/AHC	Ethanol 70%	200303	1
Pflüger/Gehe	Ethanol 70%	170619	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%	230111	1
Pflüger/Noweda	Ethanol 70%	190815	1
Pflüger/Noweda	Ethanol 70%	200409	1
Pflüger/Phönix	Ethanol 70%	190430	1
Pflüger/Phönix	Ethanol 70%	200319	1
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
Phoenix	Ethanol 70%	7027032	1
Phoenix	Ethanol 70%	7027103	1
Phoenix	Ethanol 70%	7029082	1
Phönix/Kremer	Ethanol 70%	160711	1
Phönix/Kremer	Ethanol 70%	180525	1
Phönix/Otto Fischar	Ethanol 70%	7029082	1
PHÖNIX	Ethanol 70%	171025	1
PHÖNIX	Ethanol 70%	171211	1
Phönix	Ethanol 70%	351213	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

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Supplier	Substance	Batch	Spectra
Post-Apotheke 15.01.2014	Ethanol 70%	15012044	1
Post-Apotheke	Ethanol 70%	1414A-02320	1
Purren Apotheke	Ethanol 70%	17043	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%	2615l-07145	1
Rondell Apotheke	Ethanol 70%	2616M-02320	1
Rondell Apotheke	Ethanol 70%	3414M-02320	1
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
Rosenapotheke	Ethanol 70%	2317E-07095	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
Sanacorp/Pflüger	Ethanol 70%	170906	1
Sanacorp	Ethanol 70%	130124	1
Sanacorp	Ethanol 70%	702003D	1
Sanacorp	Ethanol 70%	7020075	1
Sanacorp	Ethanol 70%	7028081	3
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
St. Martin Apotheke Ger…	Ethanol 70%	2822I-02320	2
St. Martin Apotheke Ger…	Ethanol 70%	4322l-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

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Supplier	Substance	Batch	Spectra
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
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
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
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	Ethanol 70%		4
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	Ethanol 70%	40331/52La	1
Wolf-Apotheke	Ethanol 70%	4321E-02320	1
Wolf-Apotheke-Defektur	Ethanol 70%	70818/50Hk	1

- 14 682 spectra from 1150 *Apo-Ident* customers from a total of 4462 batches from a further 158 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	200	0	28 355
Type B	0	160	0	25 941
Type C	0	727	24	14 682

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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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 98.9649 %)	96.8043 % (> 96.4048 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Ethanol 70%* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Orange aroma	54.35	–

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.

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	99.06
31055	31055	0.00	81.37
34101	34101	0.00	93.69
34274	34274	0.00	80.45

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 2.5-2023-04

Validated substance/substance group	**Excipial® almond oil ointment**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30720-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Excipial® almond oil ointment

Special notes

When selecting the *Excipial® almond oil ointment* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Excipial® almond oil ointment	5	3	65

Second-stage model

For differentiation of the substance/substance group *Excipial® almond oil ointment* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Excipial® almond oil ointment*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Galderma Labo…	Excipial® almond oil ointment	1774011	35584	50	not required
Spirig Pharma	Excipial® almond oil ointment	M023	30720	40	not required
Spirig Pharma	Excipial® almond oil ointment	M031	31090	40	not required
Spirig Pharma	Excipial® almond oil ointment	N012	31278	40	not required
Spirig Pharma	Excipial® almond oil ointment	R012	31757	60	not required

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 230 spectra of 5 reference samples from the substance/substance group *Excipial® almond oil ointment*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 28 325 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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.

- 110 spectra of 3 reference samples from the substance/substance group *Excipial® almond oil ointment*.

- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Galderma Laboratorium G…	Excipial® almond oil ointment	2774006	37418	30
Spirig Pharma	Excipial® almond oil ointment	S021	33209	40
Spirig Pharma	Excipial® almond oil ointment	T052	33210	40

- 25 991 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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.

- 260 spectra from 33 *Apo-Ident* customers from 66 batches from the substance/substance group *Excipial® almond oil ointment*.

- Among them are spectra of independent samples from 65 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	Excipial® almond oil ointment	16106712	1
Caelo	Excipial® almond oil ointment	20170829Ma2	1
Caelo	Excipial® almond oil ointment	20170829Ma3	1
Caelo	Excipial® almond oil ointment	LOTNO22	2
Caelo	Excipial® almond oil ointment	lotno32	1
Caelo	Excipial® almond oil ointment	V011	6
Ebert & Jacobi	Excipial® almond oil ointment	50239	1
Fiebig	Excipial® almond oil ointment	S051	1
Galderma (Spirig Pharma…	Excipial® almond oil ointment	R043	1
Galderma / Fiebig	Excipial® almond oil ointment	774009	1
Galderma / Gehe	Excipial® almond oil ointment	9774001	1
Galderma / Phönix	Excipial® almond oil ointment	9774006	1
Galderma International …	Excipial® almond oil ointment	T031	1
Galderma/Alliance	Excipial® almond oil ointment	V061	1
Galderma/Anzag	Excipial® almond oil ointment	S033	1
Galderma/Gehe	Excipial® almond oil ointment	774009	1
Galderma/Kehr	Excipial® almond oil ointment	774002	7
Galderma/Kehr	Excipial® almond oil ointment	T051	1
Galderma/Kehr	Excipial® almond oil ointment	V031	1
Galderma/Now	Excipial® almond oil ointment	50498	1
Galderma/Now	Excipial® almond oil ointment	774009	1
Galderma/Now	Excipial® almond oil ointment	8774006	1
Galderma/Now	Excipial® almond oil ointment	LOTS021	1
Galderma/Noweda	Excipial® almond oil ointment	S012	1
Galderma/Phoenix	Excipial® almond oil ointment	8774005	1
Galderma/Phoenix	Excipial® almond oil ointment	T021	1
Galderma/Phoenix	Excipial® almond oil ointment	T041	1
Galderma/Phönix	Excipial® almond oil ointment	50239	3
Galderma/Phönix	Excipial® almond oil ointment	8774007	1
Galderma/Phönix	Excipial® almond oil ointment	9774002	1
Galderma/Phönix	Excipial® almond oil ointment	R043	1
Galderma/Phönix	Excipial® almond oil ointment	S021	3
Galderma/Sanacorp	Excipial® almond oil ointment	1774002	1
Galderma	Excipial® almond oil ointment	10774009	1
Galderma	Excipial® almond oil ointment	1774002	6

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Supplier	Substance	Batch	Spectra
Galderma	Excipial® almond oil ointment	1774007	7
Galderma	Excipial® almond oil ointment	1774009	9
Galderma	Excipial® almond oil ointment	50238	2
Galderma	Excipial® almond oil ointment	50498	8
Galderma	Excipial® almond oil ointment	50696	19
Galderma	Excipial® almond oil ointment	774002	6
Galderma	Excipial® almond oil ointment	774004	15
Galderma	Excipial® almond oil ointment	774005	1
Galderma	Excipial® almond oil ointment	774006	2
Galderma	Excipial® almond oil ointment	774009	7
Galderma	Excipial® almond oil ointment	774010	11
Galderma	Excipial® almond oil ointment	774014	1
Galderma	Excipial® almond oil ointment	8774004	3
Galderma	Excipial® almond oil ointment	8774005	7
Galderma	Excipial® almond oil ointment	8774006	5
Galderma	Excipial® almond oil ointment	9774001	16
Galderma	Excipial® almond oil ointment	9774002	2
Galderma	Excipial® almond oil ointment	9774003	2
Galderma	Excipial® almond oil ointment	9774004	2
Galderma	Excipial® almond oil ointment	9774005	2
Galderma	Excipial® almond oil ointment	9774006	6
Galderma	Excipial® almond oil ointment	9774007	9
galderma	Excipial® almond oil ointment	LOTT061	3
Galderma	Excipial® almond oil ointment	LOTV011	2
Galderma	Excipial® almond oil ointment	R043	1
Galderma	Excipial® almond oil ointment	T011	1
Galderma	Excipial® almond oil ointment	T031	1
Galderma	Excipial® almond oil ointment	T051	1
Galderma	Excipial® almond oil ointment	T061	2
Galderma	Excipial® almond oil ointment	V031	9
Galderma	Excipial® almond oil ointment	V041	1
Galderma	Excipial® almond oil ointment	V042	2
Galderma	Excipial® almond oil ointment	V051	11
Galderma-Spirig	Excipial® almond oil ointment	V042-20171127Ma12	1
Junek GmbH	Excipial® almond oil ointment	774001	1
Junek GmbH	Excipial® almond oil ointment	9774002	1
Noweda	Excipial® almond oil ointment	8774004	1
Noweda	Excipial® almond oil ointment	9774003	1
Noweda	Excipial® almond oil ointment	9774005	2
Phoenix	Excipial® almond oil ointment	9774005	1
Spirg	Excipial® almond oil ointment	M032	1
Spirig / Galderma / Anzag	Excipial® almond oil ointment	V061	1
Spirig / Gehe	Excipial® almond oil ointment	LOTN022	1
Spirig /Noweda	Excipial® almond oil ointment	R012	1
Spirig /Noweda	Excipial® almond oil ointment	r021	1
Spirig Pharma AG/Noweda	Excipial® almond oil ointment	50239	1
Spirig Pharma/Nowed	Excipial® almond oil ointment	NO22	1
Spirig/AHD	Excipial® almond oil ointment	N011	1
Spirig/Noweda	Excipial® almond oil ointment	R043	1
Spirig/Phoenix	Excipial® almond oil ointment	50239	2
Spirig/Phönix	Excipial® almond oil ointment	N031	1
Spirig/Sanacorp	Excipial® almond oil ointment	LOTN011	1
Spirig	Excipial® almond oil ointment	LOTM023	1
Spirig	Excipial® almond oil ointment	MO23	1
Spirig	Excipial® almond oil ointment	N031	1
Spirig	Excipial® almond oil ointment	N032	1
Spirig	Excipial® almond oil ointment	R012	1
Spirig	Excipial® almond oil ointment	S011	1
Spirig	Excipial® almond oil ointment	S032	1

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- 15 173 spectra from 1165 *Apo-Ident* customers from a total of 4975 batches from a further 158 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 *Excipial*® *almond oil 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 *Excipial*® *almond oil 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	230	0	28 325
Type B	0	110	0	25 991
Type C	0	258	2	15 173

The substance/substance group *Excipial*® *almond oil 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 % (> 99.9637 %)	100.0000 % (> 97.3913 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 94.5455 %)
Type C	100.0000 % (> 98.9650 %)	99.2308 % (> 98.0769 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Excipial*® *almond oil ointment* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Balm Bio Nature	13.33	–
Argan oil	17.79	–
Wax ointment (stabilised)	40.48	–
White paraffin oil	55.31	–

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

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
30720	30720	0.00	30.50
31090	31090	0.00	24.92
31278	31278	0.00	25.42
31757	31757	0.00	22.72
35584	35584	0.00	19.58

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Fat ointments**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30881-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	26	31	246

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 ointmen…	41920120	35069	40	not required
Kaymogyn GmbH	Deumavan® protection ointmen…	13781119	35071	40	not required
Kaymogyn GmbH	Deumavan® protection ointmen…	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*
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

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1080 spectra of 26 reference samples from the substance/substance group *Fat ointments*. These samples are listed above in the *calibration samples* section. The reference samples come from 26 different batches.

- 27 475 spectra from a total of 578 batches from further 154 substances. These spectra were recorded by *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*

*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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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 by *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
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 ointmen…	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

- 24 951 spectra from a total of 556 batches from further 204 substances. These spectra were recorded by *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.

- 1064 spectra from 341 *Apo-Ident* customers from 260 batches from the substance/substance group *Fat ointments*.
- Among them are spectra of independent samples from 245 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	2711E-03598	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 Healtcare	Marjoram ointment	21000565001	1
Alliance Healthcare	Neribas® fat ointment	YY0431T	1
BAYER/Phönix WE:26.04.1...	Neribas® fat ointment	YY011K0	1
Bayer	Neribas® fat ointment	YY02L7L	1
Caeelo	Protegin® XN	20001749003	1
Caelo	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	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	9
Caelo	Marjoram ointment	14332202	1
Caelo	Protegin® XN	14341301	3
Caelo	Protegin® XN	14341302	1
Caelo	Marjoram ointment	15038303	1
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	1
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	5
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	5
Caelo	Marjoram ointment	17071101	10
Caelo	Protegin® XN	17256702	1
Caelo	Protegin® XN	17258702	1
Caelo	Protegin® XN	17258703	3
Caelo	Protegin® XN	17258705	1

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Supplier	Substance	Batch	Spectra
Caelo	Protegin® XN	17258707	3
Caelo	Protegin® XN	17258708	2
Caelo	Marjoram ointment	17302401	6
Caelo	Marjoram ointment	17302402	2
Caelo	Cottonwood ointment	18019902	1
Caelo	Marjoram ointment	18050901	7
Caelo	Marjoram ointment	18050902	3
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	14
Caelo	Marjoram ointment	18190101	5
Caelo	Marjoram ointment	18190102	4
Caelo	Marjoram ointment	18251602	1
Caelo	Marjoram ointment	18251603	1
Caelo	Marjoram ointment	18D11-T01-054700	1
Caelo	Marjoram ointment	19033001	18
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	15
Caelo	Marjoram ointment	20000282001	16
Caelo	Marjoram ointment	20000283002	7
Caelo	Marjoram ointment	20000283003	3
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
Caelo	Protegin® XN	20001749013	2
Caelo	Cottonwood ointment	20002385002	1
Caelo	Marjoram ointment	20003044001	5
Caelo	Marjoram ointment	20003045001	13
Caelo	Protegin® XN	20011402	1

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Supplier	Substance	Batch	Spectra
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	12
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	2
Caelo	Protegin® XN	22000510002	1
Caelo	Protegin® XN	22000510004	2
Caelo	Protegin® XN	22000510007	1
Caelo	Marjoram ointment	22003319001	2
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	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	19110201	1
Caesar & Loretz GmbH/ A…	Protegin® XN	21003187006	1
Caesar & Loretz GmbH/ A…	Protegin® XN	22000510002	1
Caesar & Loretz GmbH/ N…	Protegin® XN	18059507	1
Caesar & Loretz GmbH/Al…	Protegin® XN	21003187001	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/Je…	Protegin® XN	19110202	1
Caesar & Loretz GmbH/Je…	Marjoram ointment	20000281001	1
Caesar & Loretz GmbH/Je…	Marjoram ointment	20000282001	1
Caesar & Loretz GmbH/Je…	Marjoram ointment	20003044001	1
Caesar & Loretz GmbH/Kr…	Protegin® XN	19109001	1
Caesar & Loretz GmbH/Kr…	Protegin® XN	20001749010	1
Caesar & Loretz GmbH/Kr…	Protegin® XN	20001749013	1
Caesar & Loretz GmbH/No…	Protegin® XN	19109003	1
Caesar & Loretz GmbH/No…	Protegin® XN	20001749004	1
Caesar & Loretz GmbH/No…	Protegin® XN	20001749009	2
Caesar & Loretz GmbH/No…	Protegin® XN	21003187001	2
Caesar & Loretz GmbH/No…	Protegin® XN	21003187003	1
Caesar & Loretz GmbH	Protegin® XN	18059501	1
Caesar & Loretz GmbH	Protegin® XN	18059507	1
Caesar & Loretz GmbH	Protegin® XN	18059511	1

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Supplier	Substance	Batch	Spectra
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
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	2
Caesar & Loretz GmbH	Protegin® XN	20001749001	2
Caesar & Loretz GmbH	Protegin® XN	20001749003	6
Caesar & Loretz GmbH	Protegin® XN	20001749005	2
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	Protegin® XN	21003187003	4
Caesar & Loretz GmbH	Protegin® XN	21003187006	1
Caesar & Loretz GmbH	Protegin® XN	22000510002	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/Jenne	Marjoram ointment	220323(20000283002)	1
Cealo/Noweda	Protegin® XN	18059505	1
Cealo	Marjoram ointment	13028401	2
Cealo	Marjoram ointment	20003045001	1
Ceolo/Noweda	Protegin® XN	20001749012	1
Chiese	Asche Basis® fat ointment	33016A	1
Chiese	Asche Basis® fat ointment	63023A	1
Chiesi / Phönix	Asche Basis® fat ointment	93029A	2
Chiesi Sanacorp	Asche Basis® fat ointment	82027A	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/Noweda	Asche Basis® fat ointment	82027A	1
Chiesi/Phönix	Asche Basis® fat ointment	73025A	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
Deumavan/Phoenix	Deumavan® protection ointmen…	21710920	1
Elbdeich Apotheke ochse…	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

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Supplier	Substance	Batch	Spectra
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-T04009079	1
Fagron	Marjoram ointment	14A07-T04-009079	3
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 Healt…	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
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
GP Grenzach Produktions…	Neribas® fat ointment	YY00K7C	1
Hedinger/Phönix	Protegin® XN	18059501	1
Henry Lamotte GmbH/Hold…	Marjoram ointment	5067400	1
Henry Lamotte Oils GmbH…	Marjoram ointment	5067400	1
Henry Lamotte Oils GmbH…	Marjoram ointment	5322500	1
Henry Lamotte Oils GmbH	Marjoram ointment	5322500	1
Henry Lamotte Oils GmbH	Marjoram ointment	5563400	1
Henry Lamotte Oils	Marjoram ointment	5067400	1
Henry Lamotte	Marjoram ointment	5563400	1
Ichthyol-Gesellschaft	Protegin® XN	17258703	1
Jenapharm / Fiebig	Neribas® fat ointment	YY01TF2	1
Jenapharm /Gehe	Neribas® fat ointment	YY0282F	1
Jenapharm GmbH/AHCA	Neribas® fat ointment	YY01TF2	2
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	YYo11Ko	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	YYOOK7C	1

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Supplier	Substance	Batch	Spectra
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
Jenne	Marjoram ointment	13028302	2
Jenne	Cottonwood ointment	17057404	1
Karo Pharma / Phoenix	Neribas® fat ointment	YY04F1L	1
Karo Pharma/ Gehe	Neribas® fat ointment	YY04F1L	6
Karo Pharma/ Gehe	Neribas® fat ointment	YY04P2K	4
Karo Pharma/ Gehe	Neribas® fat ointment	YYo4P2K	1
Karo Pharma/ Sanacorp	Neribas® fat ointment	YY04P2K	1
KARO PHARMA/Gehe	Neribas® fat ointment	YY04P2K	1
Karo Pharma/Phoenix	Neribas® fat ointment	YY04P2K	1
Karo Pharma/Phönix	Neribas® fat ointment	YY054E8	1
Karo Pharma	Neribas® fat ointment	YY04F1L	2
Karo Pharma	Neribas® fat ointment	YY04P2K	1
Kaymogyn GmbH	Deumavan® protection ointmen…	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/ 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 Pharma	Neribas® fat ointment	yy0431T	1
Leo Pharma	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
Noweda	Protegin® XN	21003187002	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	YYO2L7L	1
Phoenix WE 24.04.17 -7,…	Neribas® fat ointment	YY019KR	1
phoenix/Karo Pharma	Neribas® fat ointment	YY04F1L	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
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

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Supplier	Substance	Batch	Spectra
PHÖNIX	Protegin® XN	18059501	1
Phönix	Marjoram ointment	18190001	2
Phönix	Protegin® XN	20001749004	1
PhönixWE:18.01.2017 E…	Neribas® fat ointment	YY016LP	1
Römerapo.	Neribas® fat ointment	YY01TF2	1
Sanacorp 05.10.21 EK:13…	Marjoram ointment	211019UM	1
Sanacorp, 21.03.17, 5,73EUR	Marjoram ointment	16068602	1
Sanacorp	Marjoram ointment	12081002	1
Sanacorp	Marjoram ointment	12295402	1
Sanacorp	Marjoram ointment	13095401	1
Sanacorp	Marjoram ointment	15038401	1
Sanacorp	Marjoram ointment	16257502	2
Sanacorp	Marjoram ointment	5563400	1
Spangropharm	Marjoram ointment	4961000	1
VDL	Marjoram ointment	14090002	1

- 14 369 spectra from 1133 *Apo-Ident* customers from a total of 4765 batches from a further 153 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	1080	0	27 475
Type B	0	1150	0	24 791
Type C	0	1049	15	14 369

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 % (> 99.9635 %)	100.0000 % (> 99.4444 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 99.4783 %)
Type C	100.0000 % (> 98.9649 %)	98.5902 % (> 98.3083 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Fat ointments* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
White paraffin oil	11.36	–
Lygal® head ointment N 3%	25.71	–
Wax ointment (stabilised)	26.44	–
Lygal® ointment base	36.08	–
Salicylic white paraffin 10%	58.20	–

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.

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	33.37
30926	30926	0.00	38.99
31013	31013	0.00	34.11
31112	31112	0.00	32.52
31443	31443	0.00	36.17
31475	31475	0.00	29.02
31489	31489	0.00	43.30
31858	31858	0.00	44.82
31872	31872	0.00	47.46
32473	32473	0.00	30.76
33130	33130	0.00	30.69
33131	33131	0.00	32.35
33634	33634	0.00	39.26
33921	33921	0.00	33.58
33986	33986	0.00	42.08
34783	34783	0.00	38.22
34963	34963	0.00	33.32
34966	34966	0.00	31.08
34967	34967	0.00	30.61
35069	35069	0.00	22.04
35071	35071	0.00	21.35
35346	35346	0.00	38.01
35471	35471	0.00	47.86
36144	36144	0.00	40.57
36671	36671	0.00	37.92
36744	36744	0.00	22.07

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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 2.5-2023-04

Validated substance/substance group	**Fenistil® Gel**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31045-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fenistil® Gel

Special notes

When selecting the *Fenistil® Gel* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Fenistil® Gel	3	2	0

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Fenistil® Gel*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Fenistil® Gel	U02364A	33638	40	not required
Novartis	Fenistil® Gel	N00927A	31045	40	not required
Novartis	Fenistil® Gel	R02021A	31767	60	not required

Validation samples

A total of 70 089 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 *Fenistil® Gel*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Fenistil® Gel*.
- 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
Euro OTC	Fenistil® Gel	T02415A	32787	40
Euro OTC	Fenistil® Gel	T02416A	32825	40

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 *Fenistil® Gel*.

- 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.

- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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 *Fenistil® Gel* 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 *Fenistil® Gel* 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	28 415
Type B	0	80	0	26 021
Type C	0	0	0	15 433

The substance/substance group *Fenistil® Gel* 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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Fenistil® Gel* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Sebexol® cream lotion pH 5	14.75	–
Sebexol® basic pH 5 formula basis	20.90	–
SyrSpend® SF pH4 cherry aroma	22.42	–
Hans Karrer Hydrocream MicroSilver	22.63	–
Excipial® U Hydrolotio	24.33	–
Aloe vera gel, 10x concentrated	26.43	–
Retterspitz external	27.77	–
SyrSpend® SF pH4 aroma free	29.86	–
Water	32.18	–
Wofacutan wash lotion	32.93	–
Aloe vera gel, 1:1	35.90	–
Dimeticone ointment 10% SR	36.61	–
Amciderm® Base cream	38.88	–
Abitima® clinic face cream	49.95	–
Hans Karrer Lipolotion MicroSilver	67.36	–

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

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
31045	31045	0.00	18.75
31767	31767	0.00	21.45
33638	33638	0.00	21.25

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Fennel oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31140-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	1

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 375 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Fennel 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
Taoasis	Fennel oil	2307-5296	1

- 15 432 spectra from 1165 *Apo-Ident* customers from a total of 5023 batches from a further 158 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	28 375
Type B	0	75	5	26 021
Type C	0	1	0	15 432

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 % (> 99.9638 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9511 %)	93.7500 % (> 90.0000 %)
Type C	100.0000 % (> 99.0163 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Fennel oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Anise oil, organic	15.86	–
Frankincense oil	67.57	–

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.

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	86.52
31693	31693	0.00	87.42
32795	32795	0.00	20.18
37662	37662	0.00	81.77

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Ginger oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30451-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	2	6

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 395 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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 *Ginger 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
Bombastus	Ginger oil	300690	32569	40
Bombastus	Ginger oil	22000860	36888	40
Bombastus	Ginger oil	300690	33014	40

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- 25 981 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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	697114345	1
Taoasis	Ginger oil	6971-14345	3

- 15 425 spectra from 1165 *Apo-Ident* customers from a total of 5018 batches from a further 158 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	28 395
Type B	0	120	0	25 981
Type C	0	8	0	15 425

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 % (> 99.9638 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9712 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Ginger oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Citus oil	17.79	–
Frankincense oil	19.00	–
Hyssop oil	20.47	–
Cedar wood oil	20.77	–
Vetiver bourbon oil	23.61	–
Marjoram oil	23.64	–
Angelica root oil	25.31	–
Myrtle oil	29.07	–
Lemon grass oil	29.48	–
Cypress oil	31.90	–
Immortelle oil	33.49	–
Pine silvestris oil	33.76	–
Spearmint oil	37.97	–
Carrot seed oil	38.75	–
Spruce needle oil	39.65	–
Yarrow oil	39.72	–
Dwarf pine oil	39.86	–
Silver fir oil	42.94	–
Cumin oil	44.94	–
Swiss pine oil	45.41	–
Matricaria oil, morrocan	49.35	–

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.

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	20.47
31142	31142	0.00	20.77
32270	32270	0.00	29.65
34407	34407	0.00	30.42

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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 2.5-2023-04

Validated substance/substance group	**Grapefruit oil organic / Orange oil / Blood orange oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30960-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	34

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

Calibration samples

Only spectra which have been recorded by *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 Bau…	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 70 089 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.
- 28 095 spectra from a total of 596 batches from further 157 substances. These spectra were recorded by *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 by *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.

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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

- 25 470 spectra from a total of 572 batches from further 207 substances. These spectra were recorded by *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 8 *Apo-Ident* customers from 34 batches from the substance/substance group *Grapefruit oil organic / Orange oil / Blood orange oil*.
- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
BerglandSanacorp	Orange oil	K602772	1
Bombastus	Orange oil	298756	1
Bombastus	Orange oil	302428	1
Caelo	Orange oil	19113809	1
Taoasis/Gehe	Orange oil	497J09	1
Taoasis/Taoasis	Grapefruit oil, organic	40238-123217	1
Taoasis/Taoasis	Orange oil	44583A-127488	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	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

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Supplier	Substance	Batch	Spectra
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	Grapefruit oil, organic	48566-1955	1
Taoasis	Orange oil	6193	1
Taoasis	Grapefruit oil, organic	AR18-12022-6352	1

- 15 398 spectra from 1164 *Apo-Ident* customers from a total of 4990 batches from a further 156 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	28 095
Type B	0	631	0	25 470
Type C	0	35	0	15 398

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 % (> 99.9636 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9508 %)	100.0000 % (> 99.0491 %)
Type C	100.0000 % (> 98.9663 %)	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.

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Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Grapefruit oil organic / Orange oil / Blood orange oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Citric oil	17.09	–
Mandarin oil, green	42.92	–
Lime oil	58.65	–

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.

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	44.07
31634	31634	0.00	42.18
31679	31679	0.00	46.09
31781	31781	0.00	46.85
31853	31853	0.00	36.86
33759	33759	0.00	44.52
33761	33761	0.00	43.89
33805	33805	0.00	44.98

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 2.5-2023-04

Validated substance/substance group	**Hydrophilic market-ready products**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30634-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydrophilic market-ready products; Abitima® clinic body cream; Abitima® clinic face cream; ALLERGIKA® – Face cream MED; Asche Basis® cream; Asche Basis® lotion; Base cream DVL-P; Base cream Taoasis; Dermatest base ointment; Dermatop® base cream; DMS® base cream classic; DMS® base cream high classic; DMS® base cream high classic plus; Eucerinum O/W basis; Eucerinum W/O basis; Excipial® hydro cream; Excipial® lipo cream; Excipial® U Lipolotio; Excipial® U10 Lipolotio; Fabitop® base cream; Hans Karrer Lipocream MicroSilver; Hans Karrer Lipolotion MicroSilver; Linola® body milk; Lipoderm® lotion; Neribas® cream; Neuroderm® care lotion; Neuroderm® moisturising cream

Special notes

When selecting the *Hydrophilic market-ready products* substance/substance group, the following information is displayed to the user:

- Advice: Currently no longer available. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Hydrophilic market-ready products	100	60	1236

Second-stage model

For differentiation of the substance/substance group *Hydrophilic market-ready products* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Hydrophilic market-ready products*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Actavis	Abitima® clinic body cream	110712	31058	40	not required
Actavis	Abitima® clinic body cream	051112	31061	40	not required
Actavis	Abitima® clinic body cream	070915	32997	40	not required
Actavis	Abitima® clinic body cream	331017	33969	40	not required
PUREN Pharma ...	Abitima® clinic body cream	185393	36760	40	not required
Actavis	Abitima® clinic face cream	46820	30845	40	not required
Actavis	Abitima® clinic face cream	161464	33793	40	not required
Actavis	Abitima® clinic face cream	170180	34360	40	not required
PUREN Pharma ...	Abitima® clinic face cream	22101318	36759	40	not required
Allergika	ALLERGIKA® – Face cream MED	2104020	35502	40	not required
Allergika	ALLERGIKA® – Face cream MED	2102013	35504	40	not required
Chiesi	Asche Basis® cream	03117A	30713	40	not required
Chiesi	Asche Basis® cream	22197A	30775	40	not required
Chiesi	Asche Basis® cream	24220A	31085	40	not required
Chiesi	Asche Basis® cream	14017A	36761	40	not required
Chiesi	Asche Basis® lotion	21042A	30828	40	not required
Chiesi	Asche Basis® lotion	24049A	31068	40	not required
Chiesi	Asche Basis® lotion	64082A	33737	40	not required
Koko	Base cream DVL-P	L061S22	36619	40	not required
Koko	Base cream DVL-P	L083T22	36620	40	not required
Taoasis	Base cream Taoasis	121205-2276	31041	100	not required
Taoasis	Base cream Taoasis	130124-3021	31115	40	not required
Taoasis	Base cream Taoasis	141222-4350	31578	60	not required
P&M Cosmetics	Dermatest base ointment	251115	31627	60	not required
P&M Cosmetics	Dermatest base ointment	180317	31950	60	not required
P&M Cosmetics	Dermatest base ointment	121217	33039	40	not required
P&M Cosmetics	Dermatest base ointment	040622	35149	40	not required
P&M Cosmetics	Dermatest base ointment	270623	36389	40	not required
P&M Cosmetics	Dermatest base ointment	301124	36774	40	not required
Sanofi aventis	Dermatop® base cream	3F031A	31234	40	not required
Sanofi aventis	Dermatop® base cream	5F056A	32177	40	not required
Sanofi aventis	Dermatop® base cream	1F107A	36037	40	not required
Koko	DMS® base cream classic	L026G13	31307	40	not required
Koko	DMS® base cream classic	L034H15	31869	60	not required
Koko	DMS® base cream classic	L003H16	32916	40	not required
Koko	DMS® base cream classic	L009K17	33968	40	not required
Koko	DMS® base cream classic	L002F22	36610	40	not required
Koko	DMS® base cream high classic	L010K13	31236	70	not required
Koko	DMS® base cream high classic	L032A14	31308	40	not required
Koko	DMS® base cream high classic	L041K15	31870	60	not required
Koko	DMS® base cream high classic	L014H22	36613	40	not required
Koko	DMS® base cream high classic...	L014L13	31309	40	not required

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Koko	DMS® base cream high classic…	L003L15	32178	40	not required
Koko	DMS® base cream high classic…	L103E22	36616	40	not required
Beiersdorf	Eucerinum O/W basis	41830108WA	31539	60	not required
Beiersdorf	Eucerinum O/W basis	64030208WA	33213	40	not required
Beiersdorf	Eucerinum W/O basis	31230108WA	30993	40	not required
Beiersdorf	Eucerinum W/O basis	53430208WA	32767	40	not required
Beiersdorf	Eucerinum W/O basis	83730208WA	34359	40	not required
Galderma Labo…	Excipial® hydro cream	0767004	35583	50	not required
Spirig Pharma	Excipial® hydro cream	I013	30725	40	not required
Spirig Pharma	Excipial® hydro cream	N013	31089	40	not required
Spirig Pharma	Excipial® hydro cream	T052	33208	40	not required
Galderma Labo…	Excipial® lipo cream	V051	33636	40	not required
Galderma Labo…	Excipial® lipo cream	1769001	35585	50	not required
Spirig Pharma	Excipial® lipo cream	I011	30726	40	not required
Spirig Pharma	Excipial® lipo cream	N017	31088	40	not required
Spirig Pharma	Excipial® lipo cream	R011	31520	60	not required
Spirig Pharma	Excipial® lipo cream	T081	33207	40	not required
Bios Medical …	Excipial® U Lipolotio	334288	35586	50	not required
Galderma Labo…	Excipial® U Lipolotio	T122	33270	40	not required
Spirig Pharma	Excipial® U Lipolotio	M042	30732	60	not required
Spirig Pharma	Excipial® U Lipolotio	N031	31067	40	not required
Spirig Pharma	Excipial® U Lipolotio	N085	31280	40	not required
Galderma Labo…	Excipial® U10 Lipolotio	375347	36770	40	not required
Spirig Pharma	Excipial® U10 Lipolotio	M021	30733	60	not required
Spirig Pharma	Excipial® U10 Lipolotio	N025	31066	40	not required
Spirig Pharma	Excipial® U10 Lipolotio	N047	31281	40	not required
Fontapharm	Fabitop® base cream	6RWW2	31082	40	not required
Fontapharm	Fabitop® base cream	GWWL3	31576	60	not required
Fontapharm	Fabitop® base cream	GLWD5	33221	40	not required
Fontapharm	Fabitop® base cream	052002	35813	50	20200508
Hans Karrer G…	Hans Karrer Lipocream MicroS…	15003	33194	40	not required
Hans Karrer G…	Hans Karrer Lipocream MicroS…	15005	33195	40	not required
Hans Karrer G…	Hans Karrer Lipocream MicroS…	18002	34117	40	not required
Hans Karrer G…	Hans Karrer Lipocream MicroS…	21002	35573	50	not required
Hans Karrer G…	Hans Karrer Lipocream MicroS…	22001	36724	40	not required
Hans Karrer G…	Hans Karrer Lipolotion Micro…	15003	31730	60	not required
Hans Karrer G…	Hans Karrer Lipolotion Micro…	15008	31873	60	not required
Hans Karrer G…	Hans Karrer Lipolotion Micro…	18005	34119	40	not required
Hans Karrer G…	Hans Karrer Lipolotion Micro…	22008	36728	40	not required
Hans Karrer G…	Hans Karrer Lipolotion Micro…	22007	36729	40	not required
Dr. Wolff	Linola® body milk	433240	31511	60	not required
Dr. Wolff	Linola® body milk	511750	31874	60	not required
Dr. Wolff	Linola® body milk	707930	34043	40	not required
Dr. Wolff	Linola® body milk	D43639	37419	40	not required
Spirig Pharma	Lipoderm® lotion	K057	30635	40	not required
Spirig Pharma	Lipoderm® lotion	M065	31072	40	not required
Spirig Pharma	Lipoderm® lotion	R023	31535	60	not required
Intendis	Neribas® cream	21076A	30634	40	not required
Intendis	Neribas® cream	21076A	31050	40	not required
Intendis	Neribas® cream	21076A	31095	40	not required
Infectopharm	Neuroderm® care lotion	S041204.1	31070	40	not required
Infectopharm	Neuroderm® care lotion	S031505.1	31772	60	not required
Infectopharm	Neuroderm® care lotion	S071706.1	34044	40	not required
Infectopharm	Neuroderm® care lotion	S042106.1	36608	40	not required
Infectopharm	Neuroderm® care lotion	S052215.1	37451	30	not required
Infectopharm	Neuroderm® moisturising cream	S041214.1	30722	40	not required
Infectopharm	Neuroderm® moisturising cream	S021307.1	31102	40	not required
Infectopharm	Neuroderm® moisturising cream	S101428.1	31761	60	not required
Infectopharm	Neuroderm® moisturising cream	S102210.1	37415	30	not required
Infectopharm	Neuroderm® moisturising cream	S112119.1	37452	30	not required

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 4530 spectra of 102 reference samples from the substance/substance group *Hydrophilic market-ready products*. These samples are listed above in the *calibration samples* section. The reference samples come from 99 different batches.
- 24 025 spectra from a total of 507 batches from further 134 substances. These spectra were recorded by *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 by *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.

- 3070 spectra of 77 reference samples from the substance/substance group *Hydrophilic market-ready products*.
- Among them are spectra of independent samples from 58 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
Actavis	Abitima® clinic body cream	072013	30736	40
Actavis	Abitima® clinic body cream	040116	32999	40
Actavis	Abitima® clinic body cream	150818	34363	40
Actavis	Abitima® clinic face cream	158584	32179	40
Allergika	ALLERGIKA® – Face cream MED	2102020	35503	40
Chiesi	Asche Basis® cream	63351A	32928	40
Chiesi	Asche Basis® cream	63354A	33435	40
Chiesi	Asche Basis® cream	11002A	35536	60
Chiesi	Asche Basis® lotion	53075A	32715	40
Chiesi	Asche Basis® lotion	94106A	35470	40
Chiesi	Asche Basis® lotion	21007A	36762	40
Koko	Base cream DVL-P	L021K22	36621	40
Taoasis	Base cream Taoasis	161124-6322	32944	40
Taoasis	Base cream Taoasis	SAP3466-3139	37690	40
P&M Cosmetics	Dermatest base ointment	120911	30737	40
P&M Cosmetics	Dermatest base ointment	070615	31053	20
P&M Cosmetics	Dermatest base ointment	231115	31288	40
P&M Cosmetics	Dermatest base ointment	260820	34032	40
Sanofi aventis	Dermatop® base cream	5F057A	32717	40
Sanofi aventis	Dermatop® base cream	7F069A	33966	40

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Supplier	Substance	Batch	Sample ID	Spectra
Koko	DMS® base cream classic	L003E16	32788	40
Koko	DMS® base cream classic	L077T22	36611	40
Koko	DMS® base cream classic	L052H22	36612	40
Koko	DMS® base cream high classic	L037K16	33433	40
Koko	DMS® base cream high classic	L064S22	36614	40
Koko	DMS® base cream high classic	L032K22	36615	40
Koko	DMS® base cream high classic…	L018D16	32827	40
Koko	DMS® base cream high classic…	L028T22	36617	40
Koko	DMS® base cream high classic…	L110H022	36618	40
Beiersdorf	Eucerinum O/W basis	94830308WA	35474	40
Beiersdorf	Eucerinum W/O basis	72630108WA	33629	40
Galderma Laboratorium G…	Excipial® hydro cream	1767002	36766	40
Spirig Pharma	Excipial® hydro cream	50235	33982	40
Galderma Laboratorium G…	Excipial® lipo cream	D372	36767	40
Galderma Laboratorium G…	Excipial® U Lipolotio	V011	33298	40
Galderma Laboratorium G…	Excipial® U Lipolotio	371412	36769	40
Spirig Pharma	Excipial® U Lipolotio	T122	33204	40
Galderma Laboratorium G…	Excipial® U10 Lipolotio	339855	35587	50
Spirig Pharma	Excipial® U10 Lipolotio	T072	33205	40
Spirig Pharma	Excipial® U10 Lipolotio	50393	33980	40
Fontapharm	Fabitop® base cream	GRWW1	30835	40
Fontapharm	Fabitop® base cream	GLWD4	33869	40
Hans Karrer GmbH	Hans Karrer Lipocream MicroS…	17001	33196	40
Hans Karrer GmbH	Hans Karrer Lipocream MicroS…	16002	33197	40
Hans Karrer GmbH	Hans Karrer Lipocream MicroS…	22002	36725	40
Hans Karrer GmbH	Hans Karrer Lipolotion Micro…	16005	32753	40
Hans Karrer GmbH	Hans Karrer Lipolotion Micro…	18004	34118	40
Hans Karrer GmbH	Hans Karrer Lipolotion Micro…	21008	35572	50
Dr. Wolff	Linola® body milk	606430	32765	40
Dr. Wolff	Linola® body milk	609202	33258	40
Spirig Pharma	Lipoderm® lotion	V012	33248	40
Spirig Pharma	Lipoderm® lotion	V042	33985	40
Jenapharm	Neribas® cream	YY01FX3	33289	40
Jenapharm	Neribas® cream	YY01X64	33951	40
Karo Pharma GmbH	Neribas® cream	YY04EYL	35478	40
Infectopharm	Neuroderm® care lotion	S111514.1	32740	40
Infectopharm	Neuroderm® care lotion	S081610.1	33286	40
Infectopharm	Neuroderm® care lotion	S052214.1	37416	30
Infectopharm	Neuroderm® moisturising cream	S051612.1	32905	40
Actavis	Abitima® clinic body cream	040116	33791	40
Actavis	Abitima® clinic face cream	158584	32723	40
Actavis	Abitima® clinic face cream	158584	32998	40
Chiesi	Asche Basis® lotion	53075A	32926	40
Taoasis	Base cream Taoasis	161124-6322	32945	40
Koko	DMS® base cream classic	L003E16	32826	40
Koko	DMS® base cream high classic	L003H16	32789	40
Koko	DMS® base cream high classic	L037K16	33434	40
Beiersdorf	Eucerinum O/W basis	64030208WA	33212	40
Beiersdorf	Eucerinum O/W basis	64030208WA	33850	40
Beiersdorf	Eucerinum W/O basis	72630108WA	33922	40
Spirig Pharma	Excipial® hydro cream	I013	30836	40
Spirig Pharma	Excipial® hydro cream	N013	31277	40
Galderma Laboratorium G…	Excipial® lipo cream	V051	33637	40
Spirig Pharma	Excipial® lipo cream	N017	31276	40
Spirig Pharma	Excipial® U Lipolotio	T122	33269	40
Infectopharm	Neuroderm® moisturising cream	S051612.1	32906	40
Infectopharm	Neuroderm® moisturising cream	S112119.1	36606	20

- 23 031 spectra from a total of 522 batches from further 184 substances. These spectra were recorded by *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.

- 4143 spectra from 523 *Apo-Ident* customers from 1276 batches from the substance/substance group *Hydrophilic market-ready products*.

- Among them are spectra of independent samples from 1143 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Asche Basis® lotion	23009a	1
	Asche Basis® cream	24021B	1
	Neribas® cream	YY02H20	1
/Sanacorp	Base cream Taoasis	180718-7100	4
>Beiersdorf	Eucerinum W/O basis	94930308	1
01.	Asche Basis® cream	12004A	1
A.H.D.	Abitima® clinic body cream	260515	2
Abitima / Gehe	Abitima® clinic body cream	251118	1
Abitima	Abitima® clinic body cream	52015/051112	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 body cream	110712	1
Actavis / Gehe	Abitima® clinic face cream	161904	3
Actavis / Noweda	Abitima® clinic face cream	142371	1
Actavis Deutschland GmbH	Abitima® clinic body cream	121115	1
Actavis Deutschland GmbH	Abitima® clinic body cream	31015	1
Actavis Deutschland GmbH	Abitima® clinic body cream	350313	2
Actavis Group PTC	Abitima® clinic body cream	260515	1
actavis group	Abitima® clinic face cream	161468	1
Actavis/ Gehe	Abitima® clinic body cream	60513	1
Actavis/ Phönix	Abitima® clinic body cream	100517	2
Actavis/	Abitima® clinic body cream	21015	1
actavis/ebert	Abitima® clinic body cream	110712	1
actavis/Gehe	Abitima® clinic body cream	110712	2
actavis/Gehe	Abitima® clinic body cream	112015	1
Actavis/Gehe	Abitima® clinic body cream	120119	2
Actavis/GEHE	Abitima® clinic face cream	148051	1
Actavis/Gehe	Abitima® clinic face cream	148495	1
Actavis/Gehe	Abitima® clinic body cream	51112	1
actavis/Gehe	Abitima® clinic body cream	60513	1
Actavis/Gehe	Abitima® clinic body cream	81013	1
Actavis/Noweda	Abitima® clinic face cream	161423	1
Actavis/Noweda	Abitima® clinic body cream	21015	1
Actavis/Phönix	Abitima® clinic face cream	159274	2
actavis/Phönix	Abitima® clinic face cream	164225	1
Actavis/Phönix	Abitima® clinic face cream	164225	1
Actavis/Sanacorp	Abitima® clinic body cream	110712	1
Actavis/Sanacorp	Abitima® clinic body cream	241118	1
Actavis	Abitima® clinic body cream	10915	4
actavis	Abitima® clinic body cream	110517	1
Actavis	Abitima® clinic body cream	131115	1
actavis	Abitima® clinic body cream	140113	1

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Supplier	Substance	Batch	Spectra
actavis	Abitima® clinic face cream	148495	1
actavis	Abitima® clinic face cream	148496	2
actavis	Abitima® clinic face cream	150202	1
actavis	Abitima® clinic face cream	150203	2
Actavis	Abitima® clinic face cream	160670	1
actavis	Abitima® clinic body cream	20912	2
Actavis	Abitima® clinic body cream	20912	1
Actavis	Abitima® clinic body cream	31015	2
Actavis	Abitima® clinic body cream	31114	2
Actavis	Abitima® clinic body cream	32018	1
actavis	Abitima® clinic body cream	60513	2
actavis	Abitima® clinic body cream	70513	1
Aenov Groupe	Asche Basis® lotion	40000200790	1
Aenova / Noweda	Asche Basis® cream	62343A	1
Aenova	Asche Basis® lotion	93102A	1
AEP/Chiesi	Asche Basis® lotion	94105A	2
AHD/Chiesi	Asche Basis® cream	11001A	1
AHD/Chiesi	Asche Basis® cream	11002A	1
AHD/Chiesi	Asche Basis® cream	2457A	1
AHD/Chiesi	Asche Basis® cream	4005A	1
AHD/Chiesi	Asche Basis® cream	92436A	1
AHD/Chiesi	Asche Basis® cream	93444A	1
AHD	Excipial® hydro cream	R011	1
AHD	Neribas® cream	YY02804	1
AHD	Neribas® cream	YY02H20	1
AHD	Neribas® cream	YY02L84	1
AHD	Neribas® cream	YY02TTH	1
AHD	Neribas® cream	YY0431J	1
AHD	Neribas® cream	YY0431K	1
All.Heal./Chiesi	Asche Basis® cream	24218A	1
Alliance Healthcare	Neuroderm® moisturising cream		2
Alliance Healthcare	Asche Basis® cream	33237A	1
Alliance Healthcare	Asche Basis® cream	33240A	1
Alliance Healthcare	Asche Basis® lotion	63981A	1
Alliance Healthcare	Asche Basis® lotion	73087A	1
Alliance Healthcare	Asche Basis® lotion	73089A	1
Alliance Healthcare	Asche Basis® lotion	82094A	2
Alliance Healthcare	Asche Basis® lotion	91098A	3
Alliance Healthcare	Asche Basis® lotion	91099A	1
Alliance Healthcare	Asche Basis® lotion	92100A	3
Alliance Healthcare	Excipial® lipo cream	M045	1
Alliance/Beiersdorf	Eucerinum W/O basis	94930208	2
Alliance/Galderma	Excipial® U Lipolotio	169853	1
Alliance/Spirig	Excipial® hydro cream	NO43	1
Alliance	Asche Basis® cream	11002A	1
Alliance	Asche Basis® cream	24022A	1
Alliance	Asche Basis® cream	31023A	1
Allianz Healthcare	Eucerinum W/O basis	64030108wa	1
Anzag/ Chiesi GmbH	Asche Basis® cream	42272A	1
Anzag/ Chiesi GmbH	Asche Basis® cream	42273A	1
Anzag/ Chiesi	Asche Basis® cream	42269A	1
Anzag/ Chiesi	Excipial® lipo cream	LOTR012	2
Anzag	Excipial® hydro cream	1767002	1
Anzag	Asche Basis® cream	23204A	1
APL Swift / Phoenix	Abitima® clinic face cream	171873	1
APL swift Service/AHD	Abitima® clinic body cream	251118	1
APL swift Service/Sanac...	Abitima® clinic body cream	90118	1
APL Swift Service	Abitima® clinic body cream	130319	2
APL Swift Service	Abitima® clinic face cream	21101170	1
APL Swift Services (Mal...	Abitima® clinic body cream	130319	1

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Supplier	Substance	Batch	Spectra
APL Swift Services	Abitima® clinic body cream	131118	1
APL Swift Services	Abitima® clinic body cream	261118	1
APL Swift Services	Abitima® clinic body cream	92021	1
APL Swift/ Phö	Abitima® clinic body cream	131118	1
APL Swift/Gehe	Abitima® clinic face cream	174418	2
APL Swift/Gehe	Abitima® clinic face cream	20101761	1
apomix	Dermatest base ointment	280821	1
apomix	Asche Basis® cream	92433A	1
Artesan	Fabitop® base cream	GLWD4	1
Artesan	Fabitop® base cream	GLWW5	1
Asche Chiesi/Alliance	Asche Basis® cream	71374A	1
Asche Chiesi/Alliance	Asche Basis® lotion	73087A	1
Astellas Pharma	Abitima® clinic body cream	190213	1
Audor Pharma	Excipial® hydro cream	V072	1
Baiersdorf	Eucerinum W/O basis	24830208WA	1
Baiersdorf	Eucerinum W/O basis	41839108WA	1
Baiersdorf	Eucerinum W/O basis	43430208WA	1
Balkanpharma	Abitima® clinic body cream	90118	2
Bayer/ Sanacorp	Neribas® cream	YY002L6	1
BDF / Gehe	Eucerinum W/O basis	83730208WA	1
BDF / Noweda	Eucerinum W/O basis	43430208WA	1
BDF / Sanacorp	Eucerinum W/O basis	21430108WA	1
BDF	Eucerinum W/O basis	31230108WA	1
BDF	Eucerinum W/O basis	41830108WA	1
Beiersdor	Eucerinum W/O basis	541830108WA	1
Beiersdorf / Alliance h...	Eucerinum W/O basis	72630108WA	1
Beiersdorf / Alliance h...	Eucerinum W/O basis	83730208WA	1
Beiersdorf / Alliance h...	Eucerinum W/O basis	949301018	1
Beiersdorf / Alliance h...	Eucerinum W/O basis	94930308	1
Beiersdorf / Fiebig	Eucerinum W/O basis	72630108WA	1
Beiersdorf / Gehe	Eucerinum W/O basis	83730208WA	1
Beiersdorf / Gehe	Eucerinum W/O basis	94930108	1
Beiersdorf / Noweda	Eucerinum W/O basis	83730208WA	1
Beiersdorf / Noweda	Eucerinum O/W basis	84030208WA	1
Beiersdorf / Noweda	Eucerinum O/W basis	94830108WA	1
Beiersdorf / Noweda	Eucerinum W/O basis	94930308	1
Beiersdorf / Phoenix	Eucerinum W/O basis	80330108WA	1
Beiersdorf / Phönix	Eucerinum W/O basis	53430208WA	1
Beiersdorf / Sanacorp	Eucerinum W/O basis	94930208	1
Beiersdorf /AHC	Eucerinum W/O basis	83730208WA	1
Beiersdorf /Sanacorp	Eucerinum W/O basis	83730208WA	1
Beiersdorf AG / Allianc...	Eucerinum O/W basis	64030208WA	1
Beiersdorf AG / Gehe	Eucerinum W/O basis	83730208WA	2
Beiersdorf AG / Gehe	Eucerinum W/O basis	83730308WA	1
Beiersdorf AG/ Alliance...	Eucerinum O/W basis	80230108WA	1
Beiersdorf AG/Kehr	Eucerinum O/W basis	84030108WA	2
Beiersdorf AG/Noweda	Eucerinum W/O basis	31230108WA	1
Beiersdorf AG/Noweda	Eucerinum O/W basis	53430208WA	1
Beiersdorf AG	Eucerinum O/W basis	2483030308WA	1
Beiersdorf AG	Eucerinum O/W basis	24830308WA	1
Beiersdorf AG	Eucerinum W/O basis	32930208WA	3
Beiersdorf AG	Eucerinum W/O basis	34930308WA	1
Beiersdorf AG	Eucerinum W/O basis	3730208WA	1
Beiersdorf AG	Eucerinum W/O basis	41830108WA	1
Beiersdorf AG	Eucerinum W/O basis	51630108WA	7
Beiersdorf AG	Eucerinum W/O basis	53630108WA	1
Beiersdorf AG	Eucerinum W/O basis	64030108WA	1
Beiersdorf AG	Eucerinum O/W basis	64030208WA	1
Beiersdorf AG	Eucerinum W/O basis	72630108WA	1
Beiersdorf AG	Eucerinum O/W basis	80230108WA	1

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Supplier	Substance	Batch	Spectra
Beiersdorf AG	Eucerinum W/O basis	80330108WA	6
Beiersdorf AG	Eucerinum W/O basis	83730208WA	1
Beiersdorf AG	Eucerinum O/W basis	84030208WA	2
Beiersdorf AG	Eucerinum O/W basis	94830108WA	1
Beiersdorf AG	Eucerinum W/O basis	94930108	1
Beiersdorf Geilenkirchen	Eucerinum W/O basis	94930308	1
Beiersdorf Manufacturin...	Eucerinum W/O basis	83730208WA	1
Beiersdorf Manufacturin...	Eucerinum W/O basis	94930208	1
Beiersdorf,Gehe	Eucerinum O/W basis	94830108WA	1
Beiersdorf,Gehe	Eucerinum W/O basis	94930108	1
Beiersdorf/ Alliance	Eucerinum W/O basis	949330208	1
Beiersdorf/ Gehe	Eucerinum W/O basis	80330108WA	1
Beiersdorf/ Noweda	Eucerinum O/W basis	94830108WA	1
beiersdorf/ noweda	Eucerinum W/O basis	94930108	1
beiersdorf/ noweda	Eucerinum W/O basis	94930208	2
Beiersdorf/ Noweda	Eucerinum W/O basis	94930208	1
Beiersdorf/ Phoenix	Eucerinum W/O basis	64030108WA	1
Beiersdorf/ Phoenix	Eucerinum O/W basis	80230108WA	1
Beiersdorf/ Phoenix	Eucerinum O/W basis	84030208Wa	1
Beiersdorf/ Phoenix	Eucerinum O/W basis	84030208WA	1
Beiersdorf/ Sanacorp	Eucerinum W/O basis	418301087WA	1
Beiersdorf/ Sanacorp	Eucerinum W/O basis	94930308	1
Beiersdorf/ Vedono	Eucerinum W/O basis	34930308WA	1
Beiersdorf/AEP	Eucerinum W/O basis	94930208	1
Beiersdorf/AHD	Eucerinum O/W basis	51630108WA	1
Beiersdorf/AHD	Eucerinum O/W basis	64030208WA	1
Beiersdorf/AHD	Eucerinum W/O basis	83730208WA	1
Beiersdorf/Alliance Hea...	Eucerinum W/O basis	72630108WA	1
Beiersdorf/Alliance	Eucerinum W/O basis	72630108WA	1
Beiersdorf/Alliance	Eucerinum W/O basis	94930108	1
Beiersdorf/Anzag	Eucerinum W/O basis	211202(94930308)	1
Beiersdorf/Anzag	Eucerinum W/O basis	31230108WA	1
Beiersdorf/E&J	Eucerinum W/O basis	80330108WA	1
Beiersdorf/Gehe	Eucerinum O/W basis	31930108WA	1
Beiersdorf/Gehe	Eucerinum W/O basis	43430208WA	1
Beiersdorf/Gehe	Eucerinum W/O basis	64030108WA	1
Beiersdorf/Gehe	Eucerinum O/W basis	80230108WA	1
Beiersdorf/Gehe	Eucerinum W/O basis	80330108WA	1
Beiersdorf/Gehe	Eucerinum W/O basis	83730208WA	1
Beiersdorf/Gehe	Eucerinum W/O basis	83730308WA	2
Beiersdorf/Gehe	Eucerinum O/W basis	84030208WA	2
Beiersdorf/Gehe	Eucerinum O/W basis	94830108WA	2
Beiersdorf/Gehe	Eucerinum O/W basis	94830308WA	1
Beiersdorf/Gehe	Eucerinum W/O basis	94930208	1
Beiersdorf/Geibo	Eucerinum W/O basis	94930108	1
Beiersdorf/Geilenkirchen	Eucerinum W/O basis	94930208	1
Beiersdorf/Jenne	Eucerinum W/O basis	94930108	1
Beiersdorf/Kehr	Eucerinum O/W basis	53430208WA	3
Beiersdorf/Kehr	Eucerinum O/W basis	61130108WA	1
Beiersdorf/Kehr	Eucerinum W/O basis	64030108WA	1
Beiersdorf/kehr	Eucerinum O/W basis	72630108WA	1
Beiersdorf/Kehr	Eucerinum W/O basis	80330108	1
Beiersdorf/Kehr	Eucerinum O/W basis	84030108WA	3
Beiersdorf/Kehr	Eucerinum O/W basis	84030208WA	4
Beiersdorf/Kehr	Eucerinum O/W basis	94830108WA	4
Beiersdorf/Kehr	Eucerinum W/O basis	94930108	1
Beiersdorf/Kehr	Eucerinum W/O basis	94930208	1
Beiersdorf/Noweda	Eucerinum W/O basis	34930308WA	1
Beiersdorf/Noweda	Eucerinum W/O basis	41830108Wa	1
Beiersdorf/Noweda	Eucerinum W/O basis	41830108WA	2

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Supplier	Substance	Batch	Spectra
Beiersdorf/Noweda	Eucerinum W/O basis	51630108wa	1
Beiersdorf/Noweda	Eucerinum W/O basis	51630108WA	6
Beiersdorf/Noweda	Eucerinum W/O basis	53430208WA	7
Beiersdorf/Noweda	Eucerinum W/O basis	53430288WA	1
Beiersdorf/Noweda	Eucerinum W/O basis	64030108WA	2
Beiersdorf/Noweda	Eucerinum W/O basis	726300108WA	1
Beiersdorf/Noweda	Eucerinum W/O basis	72630108VVA	1
Beiersdorf/Noweda	Eucerinum W/O basis	72630108WA	1
Beiersdorf/Noweda	Eucerinum W/O basis	80330108WA	2
Beiersdorf/Noweda	Eucerinum W/O basis	83730208WA	2
Beiersdorf/Noweda	Eucerinum W/O basis	83730308WA	3
Beiersdorf/Noweda	Eucerinum O/W basis	84030108WA	1
Beiersdorf/Noweda	Eucerinum O/W basis	94830308WA	1
Beiersdorf/Noweda	Eucerinum W/O basis	94930108	2
Beiersdorf/Noweda	Eucerinum W/O basis	94930208	6
Beiersdorf/Phoenix	Eucerinum W/O basis	34930308WA	1
Beiersdorf/Phoenix	Eucerinum W/O basis	51630108WA	1
Beiersdorf/Phoenix	Eucerinum W/O basis	83730206WA	2
Beiersdorf/Phoenix	Eucerinum W/O basis	94920208	1
Beiersdorf/Phoenix	Eucerinum W/O basis	94930108	1
Beiersdorf/Phoenix	Eucerinum W/O basis	94930108WA	1
Beiersdorf/Phönix	Eucerinum W/O basis	53430208WA	1
Beiersdorf/Phönix	Eucerinum W/O basis	80330108WA	2
Beiersdorf/Phönix	Eucerinum W/O basis	83730208WA	2
Beiersdorf/Phönix	Eucerinum W/O basis	94930208	1
Beiersdorf/Sanacorp	Eucerinum W/O basis	31230108WA	1
Beiersdorf/Sanacorp	Eucerinum W/O basis	83730208WA	2
Beiersdorf/Sanacorp	Eucerinum O/W basis	84030208WA	1
Beiersdorf/Sanacorp	Eucerinum W/O basis	94930108	1
Beiersdorf/Sanacorp	Eucerinum W/O basis	94930208	1
Beiersdorf/VDL	Eucerinum O/W basis	64030208WA	1
Beiersdorf	Eucerinum W/O basis	21430108WA	2
Beiersdorf	Eucerinum W/O basis	24072015A	1
beiersdorf	Eucerinum W/O basis	24830208WA	1
Beiersdorf	Eucerinum W/O basis	24830208WA	1
Beiersdorf	Eucerinum O/W basis	24830308WA	1
beiersdorf	Eucerinum W/O basis	31230108WA	1
Beiersdorf	Eucerinum W/O basis	31230108wa	1
Beiersdorf	Eucerinum W/O basis	31230108WA	1
Beiersdorf	Eucerinum O/W basis	319030108WA	1
Beiersdorf	Eucerinum W/O basis	32930208WA	5
Beiersdorf	Eucerinum W/O basis	34930308WA	6
Beiersdorf	Eucerinum W/O basis	41830108WA	3
Beiersdorf	Eucerinum W/O basis	438679	1
Beiersdorf	Eucerinum W/O basis	51630108WA	11
Beiersdorf	Eucerinum W/O basis	516301328wa	1
Beiersdorf	Eucerinum W/O basis	53430208WA	5
Beiersdorf	Eucerinum O/W basis	61130108WA	1
Beiersdorf	Eucerinum W/O basis	64030108WA	3
Beiersdorf	Eucerinum W/O basis	72630108WA	8
Beiersdorf	Eucerinum W/O basis	80330108WA	3
Beiersdorf	Eucerinum W/O basis	80339108WA	1
Beiersdorf	Eucerinum W/O basis	83730208WA	8
Beiersdorf	Eucerinum W/O basis	83730308WA	2
Beiersdorf	Eucerinum O/W basis	8373038WA	1
Beiersdorf	Eucerinum O/W basis	84030108WA	1
beiersdorf	Eucerinum W/O basis	94930108	1
Beiersdorf	Eucerinum W/O basis	94930108	3
Beiersdorf	Eucerinum W/O basis	94930208	7
beiersdorf	Eucerinum W/O basis	94930308	1

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Supplier	Substance	Batch	Spectra
Beiersdorf	Eucerinum W/O basis	94930308	1
Beiersdorf	Eucerinum W/O basis	94980208	1
BeiersdorfPhoenix	Eucerinum W/O basis	31230108WA	1
Beiersdrof/Phönix	Eucerinum W/O basis	94930208	1
Bionorica ethics	Excipial® U Lipolotio	V108	1
Bombastus	Neuroderm® moisturising cream		1
Bombastus	Base cream Taoasis	180307	1
Bombastus	Asche Basis® cream	290144	1
Bombastus	Asche Basis® lotion	74091A	1
Bombastus	Asche Basis® cream	81401A	1
Caelo	Neuroderm® moisturising cream		3
Caelo	Abitima® clinic body cream	100517	1
Caelo	Dermatest base ointment	121217	1
Caelo	Eucerinum O/W basis	13730308WA	1
Caelo	Abitima® clinic face cream	146735	1
Caelo	Abitima® clinic face cream	149666	2
Caelo	Abitima® clinic face cream	161468	2
Caelo	Base cream Taoasis	170110-6322	1
Caelo	Abitima® clinic face cream	170180	1
Caelo	Base cream Taoasis	171127-7290	1
Caelo	Excipial® U Lipolotio	173048	2
Caelo	Excipial® U Lipolotio	18023004	2
Caelo	Base cream Taoasis	180924-8114	1
Caelo	Base cream Taoasis	20001006001	1
Caelo	Asche Basis® cream	20170829Ma4	1
Caelo	Eucerinum W/O basis	21430108WA	1
Caelo	Excipial® U Lipolotio	305489	1
Caelo	Asche Basis® cream	31226A	1
Caelo	Asche Basis® cream	31227A	1
Caelo	Excipial® U Lipolotio	318628	1
Caelo	Eucerinum O/W basis	31930108WA	1
Caelo	Asche Basis® lotion	32054A	1
Caelo	Asche Basis® lotion	33055A	3
Caelo	Abitima® clinic body cream	40116	1
Caelo	Dermatest base ointment	40622	4
Caelo	Asche Basis® cream	41265B	1
Caelo	Eucerinum W/O basis	41830108WA	3
Caelo	Excipial® U Lipolotio	50569	1
Caelo	Eucerinum W/O basis	51630108	1
Caelo	Eucerinum W/O basis	51630108wa	1
Caelo	Eucerinum W/O basis	51630108WA	2
Caelo	Asche Basis® cream	52306A	3
Caelo	Asche Basis® cream	52322A	3
Caelo	Asche Basis® cream	52323a	1
Caelo	Asche Basis® lotion	53072A	1
Caelo	Asche Basis® lotion	53073A	1
Caelo	Asche Basis® lotion	53075A	1
Caelo	Asche Basis® cream	53329A	1
Caelo	Asche Basis® cream	53330A	1
Caelo	Asche Basis® cream	53331A	1
Caelo	Eucerinum W/O basis	53430208WA	5
Caelo	Neuroderm® moisturising cream	6051801	1
Caelo	Asche Basis® cream	61335A	1
Caelo	Asche Basis® cream	61337A	1
Caelo	Asche Basis® cream	61338A	1
Caelo	Asche Basis® cream	61340A	1
Caelo	Asche Basis® cream	61341A	2
Caelo	Asche Basis® lotion	63078A	1
Caelo	Eucerinum W/O basis	64030108WA	2
Caelo	Eucerinum O/W basis	64030208WA	1

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Supplier	Substance	Batch	Spectra
Caelo	Asche Basis® lotion	64082a	1
Caelo	Asche Basis® lotion	64082A	3
Caelo	Asche Basis® cream	64359A	1
Caelo	Asche Basis® cream	64363A	1
Caelo	Asche Basis® cream	64364A	2
Caelo	Excipial® lipo cream	7121	1
Caelo	Asche Basis® cream	71367A	1
Caelo	Asche Basis® cream	71372A	1
Caelo	Asche Basis® cream	72380A	2
Caelo	Eucerinum W/O basis	72630108Wa	1
Caelo	Eucerinum W/O basis	72630108WA	1
Caelo	Asche Basis® lotion	73089A	1
Caelo	Asche Basis® cream	73386A	2
Caelo	Asche Basis® cream	74391A	1
Caelo	Asche Basis® cream	74398A	1
Caelo	Eucerinum W/O basis	80330108WA	1
Caelo	Asche Basis® cream	81402A	3
Caelo	Asche Basis® cream	82409A	1
Caelo	Asche Basis® cream	83411A	4
Caelo	Asche Basis® cream	83413A	1
Caelo	Asche Basis® cream	83416A	1
Caelo	Dermatop® base cream	8F074A	1
Caelo	Excipial® lipo cream	9031	1
Caelo	Asche Basis® cream	91426A	1
Caelo	Eucerinum W/O basis	94930208	1
Caelo	Excipial® lipo cream	9769004	1
Caelo	Fabitop® base cream	glwd2	1
Caelo	Fabitop® base cream	GWWL1	1
Caelo	Fabitop® base cream	GWWL3	1
Caelo	DMS® base cream high classic	L010J15	1
Caelo	DMS® base cream high classic	L047117	4
Caelo	Hans Karrer Lipocream MicroS…	LOT17001	1
Caelo	Hans Karrer Lipolotion Micro…	LOT20001	1
Caelo	Excipial® hydro cream	LOT50782	1
Caelo	Excipial® U Lipolotio	LOTS081	1
Caelo	Excipial® lipo cream	LOTSo23	1
Caelo	Excipial® U Lipolotio	LotV137	1
Caelo	Excipial® U Lipolotio	LoTV143	1
Caelo	Excipial® hydro cream	R045	1
Caelo	Excipial® U Lipolotio	R167	1
Caelo	Excipial® U Lipolotio	R186	1
Caelo	Excipial® U Lipolotio	S073	1
Caelo	Excipial® U Lipolotio	S203	1
Caelo	Excipial® U Lipolotio	S206	1
Caelo	Excipial® hydro cream	V031	1
Caelo	Excipial® lipo cream	V051	1
Caelo	Excipial® hydro cream	V071	2
Caelo	Excipial® U Lipolotio	V101	1
Caelo	Excipial® lipo cream	V112	3
Caelo	Excipial® U Lipolotio	V143	1
Caelo	Neribas® cream	yy01k94	1
Caelo	Neribas® cream	yy01kk7	1
Caelo	Neribas® cream	YY01X64	1
Caelo	Neribas® cream	yy0203H	1
Caelo	Neribas® cream	YY0203H	1
Caelo	Neribas® cream	yy02805	1
Caelo	Neribas® cream	yyo18ff	1
Caesar & Loretz GmbH / …	Asche Basis® lotion	93103A	1
Caesar & Loretz GmbH	Excipial® U Lipolotio	19065102	1
Caesar & Loretz GmbH	Asche Basis® cream	20003818001	1

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Supplier	Substance	Batch	Spectra
Caleo/Alliance	Excipial® U Lipolotio	50791	1
Chi	Asche Basis® lotion	73088A	1
Chiesa/Phoenix	Asche Basis® cream	13010A	2
Chiese / Gehe	Asche Basis® cream	74392A	1
Chiese / Gehe	Asche Basis® cream	93446A	1
Chiese/Gehe	Asche Basis® cream	72385A	1
Chiese/Phönix	Asche Basis® cream	82408A	1
Chiese	Asche Basis® cream	1449A	1
Chiese	Asche Basis® cream	24221A	1
Chiese	Asche Basis® lotion	41060A	1
Chiese	Asche Basis® cream	41259A	1
Chiesi / Alliance Healt…	Asche Basis® cream	82410A	1
Chiesi / Anzag	Asche Basis® cream	73386A	1
Chiesi / Gehe	Asche Basis® cream	13008A	1
Chiesi / Gehe	Asche Basis® cream	13010A	1
Chiesi / Gehe	Asche Basis® cream	14016A	1
Chiesi / Gehe	Neribas® cream	32097A	1
Chiesi / Gehe	Asche Basis® cream	33244A	1
Chiesi / Gehe	Asche Basis® cream	34252A	1
Chiesi / Gehe	Asche Basis® cream	41265A	1
Chiesi / Gehe	Asche Basis® cream	42273A	1
Chiesi / Gehe	Asche Basis® cream	43281A	1
Chiesi / Gehe	Asche Basis® cream	51292A	1
Chiesi / Gehe	Asche Basis® cream	52314A	1
Chiesi / Gh Jenne	Asche Basis® cream	93447A	1
Chiesi / Jenne	Asche Basis® cream	12004A	1
Chiesi / Jenne	Asche Basis® cream	22019A	1
Chiesi / Jenne	Asche Basis® cream	4003A	1
Chiesi / Kehr	Asche Basis® cream	4004A	1
Chiesi / Kehr	Asche Basis® cream	93445A	1
Chiesi / Noweda / 07.08…	Asche Basis® lotion	84095A	1
Chiesi / Noweda / 09.04…	Asche Basis® lotion	82093A	1
Chiesi / Noweda	Asche Basis® lotion	13006A	1
Chiesi / Noweda	Asche Basis® cream	13010A	1
chiesi / Noweda	Asche Basis® cream	23213A	1
Chiesi / Noweda	Asche Basis® cream	2458A	1
chiesi / Noweda	Asche Basis® cream	31222A	1
chiesi / Noweda	Asche Basis® cream	31225A	1
Chiesi / Noweda	Asche Basis® cream	33238A	1
Chiesi / Noweda	Asche Basis® cream	33246A	1
chiesi / Noweda	Asche Basis® cream	34250A	1
CHIESI / Noweda	Asche Basis® cream	51299A	3
Chiesi / Noweda	Asche Basis® cream	51300A	1
Chiesi / Noweda	Asche Basis® cream	54332A	1
Chiesi / Noweda	Asche Basis® cream	71374A	1
Chiesi / Noweda	Asche Basis® cream	72380A	1
Chiesi / Noweda	Asche Basis® cream	73386A	2
Chiesi / Noweda	Asche Basis® cream	74393A	2
Chiesi / Noweda	Asche Basis® cream	81399A	2
Chiesi / Noweda	Asche Basis® cream	84417A	1
Chiesi / Noweda	Asche Basis® cream	91426A	1
Chiesi / Noweda	Asche Basis® cream	92435A	1
Chiesi / Noweda	Asche Basis® cream	92442A	1
Chiesi / Phoenix WE: 06…	Asche Basis® cream	53325A	1
Chiesi / Phoenix	Asche Basis® cream	13009A	1
Chiesi / Phoenix	Asche Basis® cream	14017A	1
Chiesi / Phoenix	Asche Basis® cream	51300A	1
Chiesi / Phoenix	Asche Basis® cream	52323A	2
Chiesi / Phönix	Asche Basis® cream	11003A	1
Chiesi / Phönix	Asche Basis® cream	12004A	1

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Supplier	Substance	Batch	Spectra
Chiesi / Phönix	Asche Basis® cream	12006A	1
Chiesi / Phönix	Asche Basis® cream	14013A	1
Chiesi / Phönix	Asche Basis® cream	14015A	2
Chiesi / Phönix	Asche Basis® cream	1449A	1
Chiesi / Phönix	Asche Basis® cream	22020A	1
Chiesi / Phönix	Asche Basis® cream	2458A	3
Chiesi / Phönix	Asche Basis® cream	4004A	4
Chiesi / Phönix	Asche Basis® cream	84419A	2
Chiesi / Phönix	Asche Basis® cream	91425A	2
Chiesi / Phönix	Asche Basis® cream	91430A	1
Chiesi / Phönix	Asche Basis® cream	92433A	2
Chiesi / Phönix	Asche Basis® cream	92434A	2
Chiesi / Phönix	Asche Basis® cream	92437A	3
Chiesi / Phönix	Asche Basis® cream	93446A	1
Chiesi / Phönix	Asche Basis® cream	93447A	1
Chiesi / Sanacorp	Asche Basis® cream	24022A	1
Chiesi /Ebert	Asche Basis® cream	71368A	1
Chiesi /Ebert	Asche Basis® cream	73388A	1
Chiesi /Jenne	Asche Basis® cream	1449A	2
Chiesi /Jenne	Asche Basis® cream	1451A	2
Chiesi /Jenne	Asche Basis® cream	2458A	5
Chiesi /Jenne	Asche Basis® cream	2459A	1
chiesi /Jenne	Asche Basis® cream	31227a	1
Chiesi /Jenne	Asche Basis® cream	4002A	2
Chiesi /Jenne	Asche Basis® cream	4003A	2
Chiesi /jenne	Asche Basis® cream	84418A	2
Chiesi /jenne	Asche Basis® cream	84422A	4
Chiesi /Jenne	Asche Basis® cream	91427A	1
Chiesi /Jenne	Asche Basis® cream	91431A	2
Chiesi /Jenne	Asche Basis® cream	92432A	1
Chiesi /Jenne	Asche Basis® cream	92433A	1
Chiesi /Jenne	Asche Basis® cream	93445A	2
Chiesi /Jenne	Asche Basis® cream	93447A	1
Chiesi /Noweda	Asche Basis® cream	82408A	1
Chiesi /Phönix	Asche Basis® cream	91430A	1
Chiesi GmbH / AHD	Asche Basis® cream	12007A	1
Chiesi GmbH / AHD	Asche Basis® cream	13010A	1
Chiesi GmbH / Anzag	Asche Basis® cream	22196A	1
Chiesi GmbH / Anzag	Asche Basis® cream	31222A	1
Chiesi GmbH / Anzag	Asche Basis® cream	31229A	1
Chiesi GmbH / Anzag	Asche Basis® cream	31230A	1
Chiesi GmbH / Anzag	Asche Basis® cream	31231A	2
Chiesi GmbH / Anzag	Asche Basis® cream	33244A	1
Chiesi GmbH / Anzag	Asche Basis® cream	34249A	1
Chiesi GmbH / Anzag	Asche Basis® cream	41260A	1
Chiesi GmbH / Anzag	Asche Basis® cream	41261A	1
Chiesi GmbH / Anzag	Asche Basis® cream	42268A	2
Chiesi GmbH / Anzag	Asche Basis® cream	74394A	1
Chiesi GmbH / Gehe	Asche Basis® cream	73386A	1
Chiesi GmbH / Gehe	Asche Basis® cream	92436A	1
Chiesi GmbH / Gehe	Asche Basis® cream	94448a	1
Chiesi GmbH / Phönix	Asche Basis® cream	1455A	1
Chiesi GmbH / Phönix	Asche Basis® lotion	51067A	1
Chiesi GmbH / Phönix	Asche Basis® cream	93444A	1
Chiesi GmbH / Sanacorp	Asche Basis® cream	34247A	1
Chiesi GmbH Hamburg/GEHE	Asche Basis® cream	1454A	1
Chiesi GmBH/ Alliance H...	Asche Basis® cream	83415A	1
Chiesi GmbH/ Allianz He...	Asche Basis® cream	11002A	2
Chiesi GmbH/ Gehe	Asche Basis® cream	11003A	1
Chiesi GmbH/ Noweda	Asche Basis® cream	74396A	1

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Supplier	Substance	Batch	Spectra
Chiesi GmbH/ Noweda	Asche Basis® cream	84418A	1
Chiesi GmbH/ Noweda	Asche Basis® cream	84420A	1
Chiesi GmbH/ Noweda	Asche Basis® cream	91425A	1
Chiesi GmbH/ Phönix	Asche Basis® cream	11003A	4
Chiesi GmbH/AEP	Asche Basis® cream	13008A	1
Chiesi GmbH/AHD	Asche Basis® cream	1453A	1
Chiesi GmbH/AHD	Asche Basis® cream	84420A	1
Chiesi GmbH/AHD	Asche Basis® cream	91426A	1
Chiesi GmbH/AHD	Asche Basis® cream	91427A	2
Chiesi GmbH/AHD	Asche Basis® cream	91431A	1
Chiesi GmbH/AHD	Asche Basis® cream	92433A	1
Chiesi GmbH/AHD	Asche Basis® cream	92434A	1
Chiesi GmbH/AHD	Asche Basis® cream	92441A	1
Chiesi GmbH/Gehe	Asche Basis® cream		2
Chiesi GmbH/Gehe	Asche Basis® cream	11002A	1
Chiesi GmbH/Gehe	Asche Basis® cream	12005A	1
Chiesi GmbH/Gehe	Asche Basis® cream	12007A	1
Chiesi GmbH/Gehe	Asche Basis® lotion	53072A	1
Chiesi GmbH/Gehe	Asche Basis® cream	92437A	1
Chiesi GmbH/Phoenix	Asche Basis® cream	13009A	1
Chiesi GmbH/Phoenix	Asche Basis® cream	13010A	1
Chiesi GmbH/Phoenix	Asche Basis® cream	14013A	1
Chiesi GmbH/Phoenix	Asche Basis® cream	14015A	1
Chiesi GmbH/Phoenix	Asche Basis® cream	1454A	1
Chiesi GmbH/Phoenix	Asche Basis® cream	2456A	1
Chiesi GmbH/Phoenix	Asche Basis® cream	4004A	1
Chiesi GmbH/Phoenix	Asche Basis® cream	91431A	1
Chiesi GmbH/Phoenix	Asche Basis® cream	92440A	1
Chiesi GmbH/Phoenix	Asche Basis® cream	93443A	1
Chiesi GmbH/Phönix	Asche Basis® cream	13009A	1
Chiesi GmbH/Phönix	Asche Basis® cream	14015A	2
Chiesi GmbH/Phönix	Asche Basis® cream	14016A	1
Chiesi GmbH/Phönix	Asche Basis® cream	21018A	3
Chiesi GmbH/Phönix	Asche Basis® cream	22020A	6
Chiesi GmbH/Phönix	Asche Basis® cream	4002A	1
Chiesi GmbH/Phönix	Asche Basis® cream	4003A	1
Chiesi GmbH/Phönix	Asche Basis® lotion	94106A	2
Chiesi GmbH/Sanacorp	Asche Basis® cream	93446A	1
Chiesi GmbH	Asche Basis® cream	11003A	1
Chiesi GmbH	Asche Basis® lotion	11004A	1
Chiesi GmbH	Asche Basis® lotion	1107A	2
Chiesi GmbH	Asche Basis® lotion	1108A	1
Chiesi GmbH	Asche Basis® cream	12007A	1
Chiesi GmbH	Asche Basis® lotion	13005A	1
Chiesi GmbH	Asche Basis® lotion	13006A	3
Chiesi GmbH	Asche Basis® cream	13008A	1
Chiesi GMBH	Asche Basis® cream	13008A	1
Chiesi GmbH	Asche Basis® cream	14014A	1
Chiesi GmbH	Asche Basis® cream	14017A	3
Chiesi GmbH	Asche Basis® cream	1452A	1
Chiesi GmbH	Asche Basis® cream	1453A	1
Chiesi GmbH	Asche Basis® cream	1455A	1
Chiesi GmbH	Asche Basis® lotion	2001A	1
Chiesi GmbH	Asche Basis® lotion	2002A	1
Chiesi GmbH	Asche Basis® cream	22019A	1
Chiesi GmbH	Asche Basis® cream	24214A	1
Chiesi GmbH	Asche Basis® cream	2456A	3
Chiesi GmbH	Asche Basis® cream	2459A	1
Chiesi GmbH	Asche Basis® cream	3461A	1
Chiesi GmbH	Asche Basis® cream	4005A	2

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Supplier	Substance	Batch	Spectra
Chiesi GmbH	Asche Basis® cream	52309A	2
Chiesi GmbH	Asche Basis® cream	52310A	1
Chiesi GmbH	Asche Basis® cream	52319A	1
Chiesi GmbH	Asche Basis® lotion	53071A	4
Chiesi GmbH	Asche Basis® lotion	53072A	2
Chiesi GmbH	Asche Basis® lotion	53074A	1
Chiesi GmbH	Asche Basis® lotion	61076A	2
Chiesi GmbH	Asche Basis® cream	61335A	1
Chiesi GmbH	Asche Basis® lotion	63078A	2
Chiesi GmbH	Asche Basis® lotion	63079A	2
Chiesi GmbH	Asche Basis® lotion	63980A	1
Chiesi GmbH	Asche Basis® cream	64359A	1
Chiesi GmbH	Asche Basis® cream	64363A	1
Chiesi GmbH	Asche Basis® cream	64365A	1
Chiesi GmbH	Asche Basis® cream	72379A	1
chiesi gmbh	Asche Basis® cream	72380A	1
Chiesi GmbH	Asche Basis® cream	72382A	1
Chiesi GmbH	Asche Basis® lotion	73087A	1
Chiesi GmbH	Asche Basis® cream	74394A	1
Chiesi GmbH	Asche Basis® cream	81402A	1
Chiesi GmbH	Asche Basis® cream	82407A	1
chiesi gmbh	Asche Basis® cream	82410A	1
Chiesi GmbH	Asche Basis® cream	84419A	1
Chiesi GmbH	Asche Basis® cream	84422A	2
Chiesi GmbH	Asche Basis® lotion	91098A	1
Chiesi GmbH	Asche Basis® lotion	91099A	2
Chiesi GmbH	Asche Basis® cream	91426A	1
Chiesi GmbH	Asche Basis® lotion	92100A	1
Chiesi GmbH	Asche Basis® cream	92437A	3
Chiesi GmbH	Asche Basis® cream	92439A	1
Chiesi GmbH	Asche Basis® cream	92440A	2
Chiesi GmbH	Asche Basis® lotion	93102A	1
Chiesi GmbH	Asche Basis® cream	93443A	1
Chiesi GmbH	Asche Basis® cream	93447A	1
Chiesi GmbH	Asche Basis® lotion	94104A	3
Chiesi Sanacorp	Asche Basis® cream	11003A	2
Chiesi Sanacorp	Asche Basis® cream	120005A	1
Chiesi Sanacorp	Asche Basis® cream	13010A	1
Chiesi Sanacorp	Asche Basis® cream	4002A	1
Chiesi Sanacorp	Asche Basis® cream	4003A	1
Chiesi Sanacorp	Asche Basis® cream	81404A	1
Chiesi,Fa.Gehe	Asche Basis® cream		1
Chiesi,Gehe	Asche Basis® cream		1
Chiesi/ Noweda	Asche Basis® lotion	64082A	1
Chiesi/ Noweda	Asche Basis® cream	64358A	3
Chiesi/ AEP	Asche Basis® cream	1450A	1
Chiesi/ AEP	Asche Basis® cream	2457A	1
Chiesi/ AEP	Asche Basis® cream	4003A	1
Chiesi/ Alliance	Asche Basis® cream	2456A	2
Chiesi/ Fiebig	Asche Basis® cream	63356A	1
Chiesi/ Fiebig	Asche Basis® lotion	63980A	1
Chiesi/ Fiebig	Asche Basis® cream	64363A	2
Chiesi/ Fiebig	Asche Basis® cream	72376A	2
Chiesi/ Fiebig	Asche Basis® cream	74392A	1
Chiesi/ Gehe	Asche Basis® cream	12004A	2
Chiesi/ Gehe	Asche Basis® cream	13011A	1
Chiesi/ Gehe	Asche Basis® cream	1453A	1
Chiesi/ Gehe	Asche Basis® cream	2458A	2
Chiesi/ Gehe	Asche Basis® cream	4004A	1
Chiesi/ Gehe	Asche Basis® cream	52323A	1

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Supplier	Substance	Batch	Spectra
Chiesi/ Gehe	Asche Basis® cream	73386A	1
Chiesi/ Gehe	Asche Basis® cream	82410A	1
Chiesi/ Gehe	Asche Basis® cream	83411A	1
Chiesi/ Gehe	Asche Basis® cream	84424A	1
Chiesi/ Gehe	Asche Basis® cream	92435A	1
Chiesi/ Gehe	Asche Basis® cream	92436A	1
Chiesi/ GEHE	Asche Basis® lotion	93102A	1
Chiesi/ GEHE	Asche Basis® lotion	94105A	1
Chiesi/ Now	Asche Basis® cream	33240A	1
Chiesi/ Now	Asche Basis® cream	41259A	1
Chiesi/ Now	Asche Basis® cream	42273A	1
Chiesi/ Now	Asche Basis® cream	43282A	1
Chiesi/ Now	Asche Basis® cream	43283A	2
Chiesi/ Now	Asche Basis® cream	91425A	1
Chiesi/ Noweda	Asche Basis® cream	13009A	2
Chiesi/ Noweda	Asche Basis® cream	13011A	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	171215ABC/72376A	1
Chiesi/ Noweda	Asche Basis® cream	171228ABC/72376A	1
Chiesi/ Noweda	Asche Basis® cream	180219AB/72379A	1
Chiesi/ Noweda	Asche Basis® cream	2457A	2
Chiesi/ Noweda	Asche Basis® cream	4002A	1
Chiesi/ Noweda	Asche Basis® cream	4006A	1
Chiesi/ Noweda	Asche Basis® cream	51294a	1
Chiesi/ Noweda	Asche Basis® cream	52307A	1
Chiesi/ Noweda	Asche Basis® cream	71371A	1
Chiesi/ Noweda	Asche Basis® cream	73389A	1
Chiesi/ Noweda	Asche Basis® cream	84420A	1
Chiesi/ Noweda	Asche Basis® cream	91429A	1
Chiesi/ Noweda	Asche Basis® cream	92432A	2
Chiesi/ Phoenix/ 04.03....	Asche Basis® lotion	93103A	1
Chiesi/ Phoenix/ 13.11....	Asche Basis® cream	91427A	1
Chiesi/ Phoenix/ 23.10....	Asche Basis® lotion	92100A	1
Chiesi/ Phoenix/ 30.11....	Asche Basis® lotion	1108A	1
Chiesi/ Phoenix	Asche Basis® cream	14017A	2
Chiesi/ phoenix	Asche Basis® cream	33239A	1
Chiesi/ Phoenx/ 11.08.2...	Asche Basis® lotion	941044	1
Chiesi/ Phönix	Asche Basis® cream	11001A	1
Chiesi/ Phönix	Asche Basis® cream	1451A	1
Chiesi/ Phönix	Asche Basis® cream	4002A	1
Chiesi/ Phönix	Asche Basis® lotion	43066A	1
Chiesi/ Phönix	Asche Basis® cream	84421A	1
Chiesi/ Phönix	Asche Basis® lotion	91097A	1
Chiesi/ Phönix	Asche Basis® lotion	92101A	1
Chiesi/ Phönix	Asche Basis® lotion	93102A	1
Chiesi/ Phönix	Asche Basis® lotion	94104A	1
Chiesi/ Sanacorp	Asche Basis® lotion	1107A	1
Chiesi/ Sanacorp	Asche Basis® cream	12004A	2
Chiesi/ Sanacorp	Asche Basis® cream	12005A	1
Chiesi/ Sanacorp	Asche Basis® cream	12006A	1
Chiesi/ Sanacorp	Asche Basis® cream	13009A	1
Chiesi/ Sanacorp	Asche Basis® cream	13010A	2
Chiesi/ Sanacorp	Asche Basis® cream	1451A	3
Chiesi/ Sanacorp	Asche Basis® lotion	2002A	1

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Supplier	Substance	Batch	Spectra
Chiesi/ Sanacorp	Asche Basis® cream	2459A	1
Chiesi/ Sanacorp	Asche Basis® cream	4002A	1
Chiesi/ Sanacorp	Asche Basis® cream	4004A	1
Chiesi/ Sanacorp	Asche Basis® cream	84418A	2
Chiesi/ Sanacorp	Asche Basis® cream	84419A	3
Chiesi/ Sanacorp	Asche Basis® lotion	91097A	3
Chiesi/ Sanacorp	Asche Basis® cream	91425A	2
Chiesi/ Sanacorp	Asche Basis® lotion	92100A	1
Chiesi/ Sanacorp	Asche Basis® lotion	92101A	1
Chiesi/ Sanacorp	Asche Basis® cream	92432A	1
Chiesi/ Sanacorp	Asche Basis® cream	92434A	1
Chiesi/ Sanacorp	Asche Basis® lotion	93103A	2
Chiesi/ Sanacorp	Asche Basis® cream	93443A	1
Chiesi/ Sanacorp	Asche Basis® lotion	94105A	2
Chiesi/ Sanacorp	Asche Basis® lotion	94106A	3
Chiesi//Phönix	Asche Basis® cream	63354A	1
Chiesi/	Asche Basis® cream	41266A	1
Chiesi/4	Asche Basis® cream	83412A	1
Chiesi/AEP	Asche Basis® cream	71368A	1
Chiesi/AEP	Asche Basis® cream	72385A	1
Chiesi/AEP	Asche Basis® cream	73386A	2
Chiesi/AEP	Asche Basis® cream	73388A	4
Chiesi/AEP	Asche Basis® cream	74394A	1
Chiesi/AEP	Asche Basis® cream	82405A	2
Chiesi/AEP	Asche Basis® cream	84421A	1
Chiesi/AEP	Asche Basis® cream	91428A	2
Chiesi/AHCA	Asche Basis® cream	74396A	2
Chiesi/AHCA	Asche Basis® cream	82409A	2
Chiesi/AHD/ 21.12.2020/...	Asche Basis® lotion	1107A	1
Chiesi/AHD	Asche Basis® lotion	1107A	1
Chiesi/AHD	Asche Basis® lotion	24049A	1
Chiesi/AHD	Asche Basis® cream	2456A	1
Chiesi/AHD	Asche Basis® cream	31222A	1
Chiesi/AHD	Asche Basis® cream	31223A	1
Chiesi/AHD	Asche Basis® cream	31224A	1
Chiesi/AHD	Asche Basis® cream	31228A	2
Chiesi/AHD	Asche Basis® cream	32234A	1
Chiesi/AHD	Asche Basis® cream	32235A	1
Chiesi/AHD	Asche Basis® cream	33238A	1
Chiesi/AHD	Asche Basis® cream	33242A	1
Chiesi/AHD	Asche Basis® cream	34247A	1
Chiesi/AHD	Asche Basis® cream	4002A	1
Chiesi/AHD	Asche Basis® cream	81404A	1
Chiesi/AHD	Asche Basis® cream	84419A	2
Chiesi/Alliance Healthc...	Asche Basis® cream	44290A	4
Chiesi/Alliance Healthc...	Asche Basis® cream	52323A	4
Chiesi/Alliance Healthc...	Asche Basis® cream	53329A	1
Chiesi/Alliance	Asche Basis® cream	14014A	2
Chiesi/Alliance	Asche Basis® cream	1454A	1
Chiesi/Alliance	Asche Basis® cream	2456A	1
Chiesi/Alliance	Asche Basis® cream	61338A	1
Chiesi/Alliance	Asche Basis® lotion	63981A	1
Chiesi/Alliance	Asche Basis® lotion	82092A	1
Chiesi/Alliance	Asche Basis® cream	82407A	1
Chiesi/Alliance	Asche Basis® cream	93446A	1
Chiesi/Anzag	Asche Basis® cream	12005A	1
Chiesi/Anzag	Asche Basis® cream	24221A	1
Chiesi/Anzag	Asche Basis® cream	4004A	1
Chiesi/Anzag	Asche Basis® lotion	41059A	2
Chiesi/Anzag	Asche Basis® cream	43282A	1

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Supplier	Substance	Batch	Spectra
Chiesi/Anzag	Asche Basis® cream	51295A	1
Chiesi/Anzag	Asche Basis® lotion	53075A	2
Chiesi/Anzag	Asche Basis® cream	53327A	1
Chiesi/Anzag	Asche Basis® cream	53329A	1
Chiesi/Anzag	Asche Basis® cream	74398A	1
Chiesi/Anzag	Asche Basis® lotion	91097A	1
Chiesi/Anzag	Asche Basis® cream	92437A	1
Chiesi/E+J	Asche Basis® lotion	64082A	1
Chiesi/Ebert	Asche Basis® cream	11001A	1
Chiesi/Ebert	Asche Basis® cream	12004A	1
Chiesi/Ebert	Asche Basis® cream	31224A	1
Chiesi/Ebert	Asche Basis® cream	71369A	1
Chiesi/Ebert	Asche Basis® cream	72375A	1
Chiesi/Fa.Gehe	Asche Basis® lotion	53075A	1
Chiesi/Fiebig	Asche Basis® lotion	53073A	2
Chiesi/Fiebig	Asche Basis® lotion	53074A	1
Chiesi/Fiebig	Asche Basis® lotion	63980A	1
Chiesi/Fiebig	Asche Basis® lotion	73086A	1
Chiesi/Fiebig	Asche Basis® cream	733864A	1
Chiesi/Fiebig	Asche Basis® cream	74396A	1
Chiesi/Fiebig	Asche Basis® cream	81399A	1
Chiesi/Fiebig	Asche Basis® cream	81400A	2
Chiesi/Fiebig	Asche Basis® lotion	82092A	2
Chiesi/Fiebig	Asche Basis® lotion	92100A	1
Chiesi/Fiebig	Asche Basis® cream	92434A	1
Chiesi/Fiebig	Asche Basis® cream	92436A	1
Chiesi/Gehe	Asche Basis® lotion	11003A	1
Chiesi/Gehe	Asche Basis® lotion	1107A	1
Chiesi/GEHE	Asche Basis® lotion	1108A	1
Chiesi/Gehe	Asche Basis® cream	12005A	1
Chiesi/Gehe	Asche Basis® cream	12007A	1
chiesi/gehe	Asche Basis® cream	13009A	1
Chiesi/Gehe	Asche Basis® cream	13009A	1
Chiesi/Gehe	Asche Basis® cream	13011A	2
chiesi/gehe	Asche Basis® cream	14013A	1
Chiesi/Gehe	Asche Basis® cream	1451A	1
Chiesi/Gehe	Asche Basis® lotion	2001A	2
Chiesi/Gehe	Asche Basis® lotion	2002A	1
Chiesi/Gehe	Asche Basis® lotion	23047A	1
Chiesi/Gehe	Asche Basis® cream	24218A	1
Chiesi/Gehe	Asche Basis® cream	24221A	4
Chiesi/gehe	Asche Basis® cream	2457A	1
Chiesi/Gehe	Asche Basis® cream	2457A	2
Chiesi/Gehe	Asche Basis® cream	2458A	1
Chiesi/Gehe	Asche Basis® cream	31224A	1
chiesi/gehe	Asche Basis® cream	31228A	1
Chiesi/Gehe	Asche Basis® cream	32233A	1
chiesi/gehe	Asche Basis® cream	32236A	1
chiesi/gehe	Asche Basis® lotion	33056A	2
chiesi/gehe	Asche Basis® cream	33246A	2
chiesi/gehe	Asche Basis® lotion	34058A	1
Chiesi/Gehe	Asche Basis® cream	34248A	1
Chiesi/Gehe	Asche Basis® cream	34253A	1
Chiesi/Gehe	Asche Basis® cream	4003A	2
Chiesi/Gehe	Asche Basis® cream	41260A	1
Chiesi/Gehe	Asche Basis® cream	41262A	1
Chiesi/Gehe	Asche Basis® cream	42271A	1
Chiesi/Gehe	Asche Basis® cream	43278A	1
Chiesi/Gehe	Asche Basis® cream	51300A	1
Chiesi/Gehe	Asche Basis® cream	51301A	1

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Supplier	Substance	Batch	Spectra
Chiesi/Gehe	Asche Basis® cream	52307A	1
Chiesi/Gehe	Asche Basis® cream	63350A	1
Chiesi/Gehe	Asche Basis® lotion	64082A	1
Chiesi/Gehe	Asche Basis® cream	71371A	1
Chiesi/Gehe	Asche Basis® cream	72379A	1
Chiesi/Gehe	Asche Basis® cream	72381A	2
Chiesi/Gehe	Asche Basis® cream	73388A	1
Chiesi/Gehe	Asche Basis® cream	74390A	1
Chiesi/Gehe	Asche Basis® cream	81400A	1
Chiesi/Gehe	Asche Basis® cream	81401A	1
Chiesi/Gehe	Asche Basis® cream	81402A	1
Chiesi/Gehe	Asche Basis® lotion	82092A	1
Chiesi/Gehe	Asche Basis® cream	82407A	1
Chiesi/Gehe	Asche Basis® cream	82408A	2
Chiesi/Gehe	Asche Basis® cream	82409A	2
Chiesi/Gehe	Asche Basis® cream	83413A	2
Chiesi/Gehe	Asche Basis® cream	83414A	1
Chiesi/Gehe	Asche Basis® lotion	84095A	1
Chiesi/Gehe	Asche Basis® cream	84420A	1
Chiesi/Gehe	Asche Basis® lotion	91097A	1
Chiesi/Gehe	Asche Basis® cream	91425A	1
Chiesi/Gehe	Asche Basis® cream	91426A	2
Chiesi/Gehe	Asche Basis® cream	91429A	2
Chiesi/Gehe	Asche Basis® cream	91430A	2
Chiesi/Gehe	Asche Basis® cream	92432A	1
Chiesi/Gehe	Asche Basis® cream	92434A	1
Chiesi/Gehe	Asche Basis® cream	92439A	1
Chiesi/Gehe	Asche Basis® cream	92441A	1
Chiesi/Gehe	Asche Basis® cream	93447A	1
Chiesi/Gehe	Asche Basis® lotion	94106A	4
Chiesi/Gehe	Asche Basis® cream	941426A	1
Chiesi/Insel	Asche Basis® cream	74391A	1
Chiesi/Jenne	Asche Basis® cream	12006A	1
Chiesi/Jenne	Asche Basis® cream	12007A	1
Chiesi/Jenne	Asche Basis® cream	14013A	1
Chiesi/Jenne	Asche Basis® cream	14014A	1
Chiesi/Jenne	Asche Basis® cream	14016A	3
Chiesi/Jenne	Asche Basis® cream	22020A	2
Chiesi/Jenne	Asche Basis® cream	83413A	1
Chiesi/Jenne	Asche Basis® cream	84421A	2
Chiesi/Jenne	Asche Basis® cream	91429A	3
Chiesi/Kehr	Asche Basis® cream	20008410/0	1
Chiesi/Kehr	Asche Basis® cream	22020A	4
Chiesi/Kehr	Asche Basis® cream	2458A	1
Chiesi/Kehr	Asche Basis® cream	2460A	2
Chiesi/Kehr	Asche Basis® cream	81402A	2
Chiesi/Kehr	Asche Basis® cream	82409A	1
Chiesi/Kehr	Asche Basis® cream	83414A	1
Chiesi/Kehr	Asche Basis® cream	83416A	1
Chiesi/Kehr	Asche Basis® cream	84421A	2
Chiesi/Kehr	Asche Basis® cream	84422A	1
Chiesi/Kehr	Asche Basis® cream	84423A	1
Chiesi/Kehr	Asche Basis® cream	91427A	1
Chiesi/Kehr	Asche Basis® cream	91431A	1
Chiesi/Kehr	Asche Basis® cream	92432A	2
Chiesi/Kehr	Asche Basis® cream	92439A	2
Chiesi/Krieger	Asche Basis® cream		1
Chiesi/Krieger	Asche Basis® cream	1449A	1
Chiesi/Krieger	Asche Basis® cream	1452A	2
Chiesi/Krieger	Asche Basis® cream	4003A	2

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Supplier	Substance	Batch	Spectra
Chiesi/Krieger	Asche Basis® lotion	64082A	1
Chiesi/Krieger	Asche Basis® cream	64363A	1
Chiesi/Krieger	Asche Basis® cream	72379A	1
Chiesi/Krieger	Asche Basis® cream	72383A	1
Chiesi/Krieger	Asche Basis® cream	72384A	1
Chiesi/Krieger	Asche Basis® cream	74396A	1
Chiesi/Krieger	Asche Basis® cream	81402A	2
Chiesi/Krieger	Asche Basis® cream	81403A	1
Chiesi/Krieger	Asche Basis® lotion	82092A	3
Chiesi/Krieger	Asche Basis® cream	82407A	1
Chiesi/Krieger	Asche Basis® cream	82409A	1
Chiesi/Krieger	Asche Basis® cream	91427A	1
Chiesi/Krieger	Asche Basis® cream	91430A	2
Chiesi/Krieger	Asche Basis® cream	91431A	1
Chiesi/Krieger	Asche Basis® cream	92435A	1
Chiesi/Krieger	Asche Basis® cream	93444A	1
Chiesi/Lichtenheld	Asche Basis® cream	12007A	1
Chiesi/Noweda	Asche Basis® cream	12004A	3
Chiesi/Noweda	Asche Basis® cream	12005A	1
Chiesi/Noweda	Asche Basis® cream	12006A	3
Chiesi/Noweda	Asche Basis® cream	12007A	2
Chiesi/Noweda	Asche Basis® lotion	13005A	3
Chiesi/Noweda	Asche Basis® cream	13011A	2
Chiesi/Noweda	Asche Basis® cream	1450A	1
Chiesi/Noweda	Asche Basis® cream	1454A	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	22019A	1
Chiesi/Noweda	Asche Basis® cream	2456A	2
Chiesi/Noweda	Asche Basis® cream	31224A	1
Chiesi/Noweda	Asche Basis® cream	31229A	1
Chiesi/Noweda	Asche Basis® cream	31232A	1
Chiesi/Noweda	Asche Basis® cream	33237A	1
Chiesi/Noweda	Asche Basis® cream	34247A	1
Chiesi/Noweda	Asche Basis® cream	4003A	2
Chiesi/Noweda	Asche Basis® cream	41258A	1
Chiesi/Noweda	Asche Basis® cream	42275A	1
Chiesi/Noweda	Asche Basis® cream	43280A	1
Chiesi/Noweda	Asche Basis® cream	44288A	1
Chiesi/Noweda	Asche Basis® cream	52306A	2
Chiesi/Noweda	Asche Basis® cream	52318a	1
Chiesi/Noweda	Asche Basis® cream	52318A	1
Chiesi/Noweda	Asche Basis® cream	53329A	1
Chiesi/Noweda	Asche Basis® lotion	61077A	1
Chiesi/Noweda	Asche Basis® cream	6234A	1
Chiesi/Noweda	Asche Basis® cream	63347A	1
Chiesi/Noweda	Asche Basis® lotion	64082A	1
Chiesi/Noweda	Asche Basis® lotion	71083A	1
Chiesi/Noweda	Asche Basis® lotion	73089A	1
Chiesi/Noweda	Asche Basis® cream	74394A	1
Chiesi/Noweda	Asche Basis® cream	81404A	2
Chiesi/Noweda	Asche Basis® cream	82410A	1
Chiesi/Noweda	Asche Basis® cream	83412A	1
Chiesi/Noweda	Asche Basis® cream	844194	1
Chiesi/Noweda	Asche Basis® cream	84419A	1
Chiesi/Noweda	Asche Basis® cream	84424A	2
Chiesi/Noweda	Asche Basis® cream	92432A	1
Chiesi/Noweda	Asche Basis® cream	92433A	1

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Supplier	Substance	Batch	Spectra
Chiesi/Noweda	Asche Basis® cream	92434A	1
Chiesi/Noweda	Asche Basis® cream	92440A	1
Chiesi/Noweda	Asche Basis® lotion	93102A	1
Chiesi/Noweda	Asche Basis® lotion	93103A	1
Chiesi/Noweda	Asche Basis® cream	94448A	1
chiesi/Phoen	Asche Basis® cream	73388A	1
Chiesi/Phoenix	Asche Basis® cream	24215A	1
Chiesi/Phoenix	Asche Basis® cream	2456A	1
Chiesi/Phoenix	Asche Basis® cream	31225A	1
Chiesi/Phoenix	Asche Basis® cream	31227A	2
Chiesi/Phoenix	Asche Basis® cream	31229A	1
Chiesi/Phoenix	Asche Basis® cream	32233A	1
Chiesi/Phoenix	Asche Basis® cream	43278A	1
Chiesi/Phoenix	Asche Basis® lotion	52070A	1
Chiesi/Phoenix	Asche Basis® lotion	53071A	1
Chiesi/Phoenix	Asche Basis® lotion	64082A	1
Chiesi/Phoenix	Asche Basis® cream	71368A	1
Chiesi/Phoenix	Asche Basis® cream	72377A	1
Chiesi/Phoenix	Asche Basis® cream	72383A	1
Chiesi/Phoenix	Asche Basis® lotion	73086A	1
Chiesi/Phoenix	Asche Basis® cream	74390A	2
chiesi/Phoenix	Asche Basis® cream	74394A	1
Chiesi/Phoenix	Asche Basis® cream	74394A	1
Chiesi/Phoenix	Asche Basis® cream	81401A	1
chiesi/Phoenix	Asche Basis® cream	82407A	1
chiesi/Phoenix	Asche Basis® cream	83416A	1
Chiesi/Phoenix	Asche Basis® cream	84418A	1
Chiesi/Phoenix	Asche Basis® cream	92437A	2
Chiesi/Phoenix	Asche Basis® cream	92438A	1
Chiesi/Phoenix	Asche Basis® cream	93443A	1
Chiesi/Phoenix	Asche Basis® cream	93447A	1
Chiesi/Phoenix	Excipial® hydro cream	LOTV071	1
Chiesi/Phönix WE:19.05....	Asche Basis® cream	64357A	1
Chiesi/Phönix WE:20.06....	Asche Basis® cream	64362A	2
Chiesi/Phönix WE:27.05....	Asche Basis® cream	52309A	1
Chiesi/Phönix	Asche Basis® cream	11002A	2
Chiesi/Phönix	Asche Basis® cream	12004A	1
Chiesi/Phönix	Asche Basis® cream	13010A	1
Chiesi/Phönix	Asche Basis® cream	1451A	1
Chiesi/Phönix	Asche Basis® cream	1452A	1
Chiesi/Phönix	Asche Basis® cream	2456A	1
Chiesi/Phönix	Asche Basis® cream	2459A	1
Chiesi/Phönix	Asche Basis® cream	4004A	1
Chiesi/Phönix	Asche Basis® lotion	53071A	1
Chiesi/Phönix	Asche Basis® lotion	53073A	1
Chiesi/Phönix	Asche Basis® cream	53329A	1
Chiesi/Phönix	Asche Basis® cream	61334A	1
Chiesi/Phönix	Asche Basis® lotion	63078A	1
Chiesi/Phönix	Asche Basis® lotion	63981A	1
Chiesi/Phönix	Asche Basis® cream	64358A	1
Chiesi/Phönix	Asche Basis® cream	71367A	1
Chiesi/Phönix	Asche Basis® cream	72375A	1
Chiesi/Phönix	Asche Basis® cream	72385A	2
Chiesi/Phönix	Asche Basis® lotion	73086A	2
Chiesi/Phönix	Asche Basis® cream	73388A	2
Chiesi/Phönix	Asche Basis® cream	74394A	1
Chiesi/Phönix	Asche Basis® cream	81400A	1
Chiesi/Phönix	Asche Basis® cream	81401A	2
Chiesi/Phönix	Asche Basis® cream	81402A	1
Chiesi/Phönix	Asche Basis® cream	81404A	2

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Supplier	Substance	Batch	Spectra
Chiesi/phönix	Asche Basis® lotion	82092A	1
Chiesi/Phönix	Asche Basis® lotion	82092A	1
Chiesi/Phönix	Asche Basis® cream	82405A	1
Chiesi/Phönix	Asche Basis® cream	82407A	1
Chiesi/Phönix	Asche Basis® cream	83412A	4
Chiesi/Phönix	Asche Basis® cream	83416A	5
Chiesi/Phönix	Asche Basis® lotion	84095A	2
Chiesi/Phönix	Asche Basis® cream	84417A	1
Chiesi/Phönix	Asche Basis® cream	84418A	4
Chiesi/Phönix	Asche Basis® cream	84419A	3
Chiesi/Phönix	Asche Basis® cream	84420A	2
Chiesi/Phönix	Asche Basis® cream	84421A	1
Chiesi/Phonix	Asche Basis® lotion	91097A	1
Chiesi/Phönix	Asche Basis® cream	91425A	1
Chiesi/Phönix	Asche Basis® cream	91426A	2
Chiesi/Phönix	Asche Basis® cream	91427A	1
Chiesi/Phönix	Asche Basis® cream	91429A	3
Chiesi/Phönix	Asche Basis® cream	91430A	1
Chiesi/Phönix	Asche Basis® lotion	92100A	1
Chiesi/Phönix	Asche Basis® cream	92432A	1
Chiesi/Phönix	Asche Basis® cream	92434A	1
Chiesi/Phönix	Asche Basis® cream	92435A	1
Chiesi/Phönix	Asche Basis® cream	92437A	4
Chiesi/Phönix	Asche Basis® cream	92438A	1
Chiesi/Phönix	Asche Basis® cream	92441A	1
Chiesi/Phönix	Asche Basis® cream	93443A	1
Chiesi/Phönix	Asche Basis® cream	93444A	1
Chiesi/Phönix	Asche Basis® lotion	94106A	2
Chiesi/Sanacorp WE:06.0…	Asche Basis® cream	52317A	1
Chiesi/Sanacorp	Asche Basis® cream	11002A	1
chiesi/sanacorp	Asche Basis® cream	1453A	1
Chiesi/Sanacorp	Asche Basis® lotion	21007A	1
Chiesi/Sanacorp	Asche Basis® cream	2456A	1
Chiesi/Sanacorp	Asche Basis® cream	31227A	1
Chiesi/sanacorp	Asche Basis® cream	3461A	1
Chiesi/Sanacorp	Asche Basis® cream	4002A	1
Chiesi/sanacorp	Asche Basis® cream	4005A	1
Chiesi/sanacorp	Asche Basis® cream	4006A	1
Chiesi/Sanacorp	Asche Basis® cream	51305A	3
chiesi/sanacorp	Asche Basis® cream	74393A	2
Chiesi/Sanacorp	Asche Basis® cream	74394A	1
Chiesi/Sanacorp	Asche Basis® cream	82408A	1
Chiesi/Sanacorp	Asche Basis® cream	83412A	1
Chiesi/Sanacorp	Asche Basis® cream	83413A	1
Chiesi/Sanacorp	Asche Basis® cream	84418A	2
Chiesi/Sanacorp	Asche Basis® cream	84423A	1
Chiesi/Sanacorp	Asche Basis® cream	84424A	1
Chiesi/Sanacorp	Asche Basis® lotion	91097A	2
Chiesi/Sanacorp	Asche Basis® lotion	91098A	1
Chiesi/Sanacorp	Asche Basis® cream	91425A	1
Chiesi/Sanacorp	Asche Basis® cream	91426A	1
Chiesi/Sanacorp	Asche Basis® cream	92434A	1
Chiesi/Sanacorp	Asche Basis® cream	92441A	1
Chiesi/sanacorp	Asche Basis® cream	92442A	1
Chiesi/Sanacorp	Asche Basis® cream	93443A	3
Chiesi/Sanacorp	Asche Basis® cream	93446A	1
Chiesi/Spangro 13.10.21	Asche Basis® lotion	94106A	1
Chiesi/Spangro	Asche Basis® cream	4002A	1
Chiesi/V.d.L.	Asche Basis® cream	34250A	1
Chiesi/VDL	Asche Basis® cream	1455A	1

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Supplier	Substance	Batch	Spectra
Chiesi/VDL	Asche Basis® cream	92436A	1
Chiesi	Asche Basis® cream	1(81404A)	1
Chiesi	Asche Basis® cream	11001A	6
Chiesi	Asche Basis® cream	11002A	3
Chiesi	Asche Basis® cream	11003A	11
Chiesi	Asche Basis® lotion	11004A	2
Chiesi	Asche Basis® lotion	1107A	2
Chiesi	Asche Basis® cream	12004A	2
Chiesi	Asche Basis® cream	12005A	5
Chiesi	Asche Basis® cream	12006A	3
Chiesi	Asche Basis® cream	12007A	1
Chiesi	Asche Basis® lotion	13005A	2
Chiesi	Asche Basis® lotion	13006A	2
Chiesi	Asche Basis® cream	13008A	2
Chiesi	Asche Basis® cream	13009A	1
Chiesi	Asche Basis® cream	14012A	2
Chiesi	Asche Basis® cream	14013A	2
Chiesi	Asche Basis® cream	14016A	2
Chiesi	Asche Basis® cream	14178A	1
Chiesi	Asche Basis® cream	1449A	4
Chiesi	Asche Basis® cream	1450A	1
Chiesi	Asche Basis® cream	1451A	2
Chiesi	Asche Basis® cream	1453A	2
Chiesi	Asche Basis® cream	1454A	2
Chiesi	Asche Basis® cream	1455A	3
Chiesi	Asche Basis® lotion	2001A	3
Chiesi	Asche Basis® lotion	2002A	1
Chiesi	Asche Basis® lotion	21007A	1
Chiesi	Asche Basis® lotion	2100A	1
Chiesi	Asche Basis® cream	23204A	1
Chiesi	Asche Basis® cream	23206A	1
Chiesi	Asche Basis® lotion	24049A	1
Chiesi	Asche Basis® cream	24214A	2
Chiesi	Asche Basis® cream	24217A	1
Chiesi	Asche Basis® cream	24219A	1
Chiesi	Asche Basis® cream	24220A	2
Chiesi	Asche Basis® cream	2456A	2
Chiesi	Asche Basis® cream	2457A	2
Chiesi	Asche Basis® cream	2459A	2
Chiesi	Asche Basis® cream	2460A	1
Chiesi	Asche Basis® cream	30102014A	1
Chiesi	Asche Basis® cream	31227A	2
Chiesi	Asche Basis® cream	31232A	1
Chiesi	Asche Basis® lotion	32054A	2
Chiesi	Asche Basis® cream	32233A	4
Chiesi	Asche Basis® cream	32235A	1
Chiesi	Asche Basis® cream	32236A	1
Chiesi	Asche Basis® cream	33237A	1
Chiesi	Asche Basis® cream	33239A	2
Chiesi	Asche Basis® cream	33240A	1
Chiesi	Asche Basis® cream	33243A	1
Chiesi	Asche Basis® lotion	333056A	2
Chiesi	Asche Basis® cream	34248A	1
Chiesi	Asche Basis® cream	34249A	1
Chiesi	Asche Basis® cream	34250A	1
Chiesi	Asche Basis® cream	34251A	3
chiesi	Asche Basis® cream	3461A	1
Chiesi	Asche Basis® cream	3461A	2
Chiesi	Asche Basis® cream	4002A	1
Chiesi	Asche Basis® cream	4003A	5

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Supplier	Substance	Batch	Spectra
Chiesi	Asche Basis® cream	4004A	3
Chiesi	Asche Basis® cream	4005A	2
chiesi	Asche Basis® cream	4006A	1
Chiesi	Asche Basis® cream	4006A	1
Chiesi	Asche Basis® lotion	41059A	1
Chiesi	Asche Basis® cream	41258A	2
Chiesi	Asche Basis® cream	41260A	2
Chiesi	Asche Basis® cream	41261A	1
CHiesi	Asche Basis® cream	41264A	1
Chiesi	Asche Basis® lotion	42062A	2
Chiesi	Asche Basis® lotion	42063A	1
Chiesi	Asche Basis® cream	42270A	1
Chiesi	Asche Basis® cream	42271A	2
Chiesi	Asche Basis® cream	42272A	1
Chiesi	Asche Basis® cream	42275A	1
Chiesi	Asche Basis® lotion	43065A	2
Chiesi	Asche Basis® lotion	43066A	1
Chiesi	Asche Basis® cream	43262A	1
Chiesi	Asche Basis® cream	43278A	1
Chiesi	Asche Basis® cream	43279A	1
Chiesi	Asche Basis® cream	43280A	1
Chiesi	Asche Basis® cream	43283A	1
Chiesi	Asche Basis® cream	43287A	2
Chiesi	Asche Basis® cream	44288A	1
Chiesi	Asche Basis® cream	44290A	1
Chiesi	Asche Basis® lotion	46082A	1
Chiesi	Asche Basis® lotion	51067A	1
Chiesi	Asche Basis® cream	51294A	1
Chiesi	Asche Basis® cream	51296A	2
Chiesi	Asche Basis® cream	51300A	4
Chiesi	Asche Basis® cream	51305A	2
Chiesi	Asche Basis® lotion	52069A	1
Chiesi	Asche Basis® cream	52307A	2
Chiesi	Asche Basis® cream	52308A	4
Chiesi	Asche Basis® cream	52309A	1
Chiesi	Asche Basis® cream	52310A	3
Chiesi	Asche Basis® cream	52315A	1
Chiesi	Asche Basis® cream	52322A	1
Chiesi	Asche Basis® lotion	53072A	2
Chiesi	Asche Basis® lotion	53073A	2
Chiesi	Asche Basis® lotion	53074A	3
Chiesi	Asche Basis® lotion	53075A	2
Chiesi	Asche Basis® cream	53326A	1
Chiesi	Asche Basis® cream	53329A	1
Chiesi	Asche Basis® cream	53330A	1
Chiesi	Asche Basis® cream	53331A	2
Chiesi	Asche Basis® cream	54332A	2
Chiesi	Asche Basis® lotion	61076A	1
Chiesi	Asche Basis® lotion	61077A	1
Chiesi	Asche Basis® cream	61338A	1
Chiesi	Asche Basis® cream	62343A	3
Chiesi	Asche Basis® cream	62344A	1
Chiesi	Asche Basis® cream	63347A	5
Chiesi	Asche Basis® cream	63350A	1
Chiesi	Asche Basis® cream	63351A	1
Chiesi	Asche Basis® cream	63354A	2
Chiesi	Asche Basis® cream	63355A	1
Chiesi	Asche Basis® lotion	63980A	2
Chiesi	Asche Basis® lotion	63981A	1
Chiesi	Asche Basis® lotion	64082A	1

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Supplier	Substance	Batch	Spectra
Chiesi	Asche Basis® cream	64357A	3
Chiesi	Asche Basis® cream	64359A	1
Chiesi	Asche Basis® cream	64360A	3
Chiesi	Asche Basis® cream	64362A-20170704Ma4	1
Chiesi	Asche Basis® cream	64364A	1
Chiesi	Asche Basis® lotion	71083A	1
Chiesi	Asche Basis® cream	71370A	4
Chiesi	Asche Basis® cream	71372A	1
chiesi-	Asche Basis® cream	71372A20171127Ma13	1
Chiesi	Asche Basis® cream	71373A	1
chiesi	Asche Basis® cream	71374A	1
Chiesi	Asche Basis® cream	71374A	1
Chiesi	Asche Basis® cream	72375A	4
chiesi-	Asche Basis® cream	72376A-20180830Ma8	1
Chiesi	Asche Basis® cream	72378A	1
Chiesi	Asche Basis® cream	72379A	2
Chiesi	Asche Basis® cream	72380A	1
Chiesi	Asche Basis® cream	72382A	2
Chiesi	Asche Basis® cream	72383A	1
Chiesi	Asche Basis® cream	72384A	2
Chiesi	Asche Basis® cream	72388A	1
Chiesi	Asche Basis® lotion	73085A	1
Chiesi	Asche Basis® lotion	730874	1
Chiesi	Asche Basis® lotion	73088a	1
Chiesi	Asche Basis® lotion	73088A	3
Chiesi	Asche Basis® cream	73387A	2
Chiesi	Asche Basis® cream	73389A	1
Chiesi	Asche Basis® cream	74390A	3
Chiesi	Asche Basis® cream	74391A	1
Chiesi	Asche Basis® cream	74392A	2
Chiesi	Asche Basis® cream	74393A	2
Chiesi	Asche Basis® cream	74396A	1
Chiesi	Asche Basis® cream	74397A	2
Chiesi	Asche Basis® cream	74398A	4
Chiesi	Asche Basis® lotion	75085A	1
Chiesi	Asche Basis® cream	81399A	2
Chiesi	Asche Basis® cream	81400A	5
Chiesi	Asche Basis® cream	81401A	5
Chiesi	Asche Basis® cream	81402A	2
Chiesi	Asche Basis® cream	81403A	1
Chiesi	Asche Basis® cream	81404A	1
Chiesi	Asche Basis® lotion	82092A	1
Chiesi	Asche Basis® lotion	82094A	1
Chiesi	Asche Basis® cream	82405A	3
chiesi	Asche Basis® cream	82407A	1
Chiesi	Asche Basis® cream	82407A	5
Chiesi	Asche Basis® cream	82409A	1
Chiesi	Asche Basis® cream	82410A	1
Chiesi	Asche Basis® cream	83411A	1
Chiesi	Asche Basis® cream	83412A	2
chiesi	Asche Basis® cream	83413A	1
Chiesi	Asche Basis® cream	83413A	5
Chiesi	Asche Basis® cream	83414A	3
Chiesi	Asche Basis® cream	83415A	1
Chiesi	Asche Basis® cream	83416A	3
chiesi	Asche Basis® lotion	84095A	1
Chiesi	Asche Basis® lotion	84096A	1
Chiesi	Asche Basis® cream	84413A	1
Chiesi	Asche Basis® cream	84417A	2
Chiesi	Asche Basis® cream	84418A	1

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Supplier	Substance	Batch	Spectra
Chiesi	Asche Basis® cream	84419A	2
Chiesi	Asche Basis® cream	84421A	2
chiesi	Asche Basis® cream	84422A	1
Chiesi	Asche Basis® cream	84422A	1
chiesi	Asche Basis® cream	84423A	1
Chiesi	Asche Basis® cream	84423A	3
Chiesi	Asche Basis® cream	84424A	2
Chiesi	Asche Basis® cream	91425A	3
Chiesi	Asche Basis® cream	91426A	6
Chiesi	Asche Basis® cream	91427A	1
Chiesi	Asche Basis® cream	91428A	1
Chiesi	Asche Basis® cream	91429A	2
Chiesi	Asche Basis® cream	91430A	1
Chiesi	Asche Basis® cream	91431A	3
Chiesi	Asche Basis® lotion	92101A	3
Chiesi	Asche Basis® cream	92432A	2
Chiesi	Asche Basis® cream	92433A	2
Chiesi	Asche Basis® cream	92434A	4
Chiesi	Asche Basis® cream	92436A	2
Chiesi	Asche Basis® cream	92437A	4
Chiesi	Asche Basis® cream	92438A	1
Chiesi	Asche Basis® cream	92439A	4
Chiesi	Asche Basis® cream	92441A	4
Chiesi	Asche Basis® cream	92442A	1
Chiesi	Asche Basis® cream	92A36A	1
Chiesi	Asche Basis® cream	93443A	4
Chiesi	Asche Basis® cream	93444A	2
Chiesi	Asche Basis® cream	93445A	1
Chiesi	Asche Basis® cream	93446A	6
Chiesi	Asche Basis® lotion	94104A	3
Chiesi	Asche Basis® lotion	94105A	3
Chiesi	Asche Basis® lotion	94106A	1
chiesi	Asche Basis® cream	94448A	1
Chiesi	Asche Basis® cream	94448AI	1
Chiesi	Asche Basis® cream	94448AII	1
Chiesi	Excipial® U Lipolotio	S116	1
Chiesie GmbH/Jenne	Asche Basis® cream	11002A	1
Chiesie GmbH/Jenne	Asche Basis® cream	2456A	2
Chiesie GmbH/Phönix	Asche Basis® cream	4002A	1
Chiesie GmbH/Phönix	Asche Basis® cream	83415A	1
Chiesie GmbH/Phönix	Asche Basis® cream	91425A	2
Chiesie GmbH/Phönix	Asche Basis® cream	92432A	1
Chiesie/Anzag	Asche Basis® lotion	32054A	1
Chiesie	Asche Basis® cream	84417A	1
Chiesie	Asche Basis® cream	92436A	1
Chiesie	Asche Basis® cream	92439A	1
Chiesi-Fa.Gehe 19.6.18	Asche Basis® cream	74391A-20180830Ma7	1
Chiesi-Fa.Gehe 19.7.18	Asche Basis® lotion	74090A-20180830Ma10	1
Chiesi-Fa.Gehe	Asche Basis® lotion	64082A-20180112Ma3	1
Chiesi-Fa.Gehe	Asche Basis® cream	71372A	1
Chiesi-Fa.Gehe	Asche Basis® lotion	73086A-20180206Ma8	1
Chiesi-Fa.Gehe	Asche Basis® lotion	73087A-20180206Ma9	1
Chiesi-Fa.Gehe	Asche Basis® cream	81401A-A20190115Ma11	1
Chiesi-Fa.Gehe	Asche Basis® lotion	82093A-A20181115Ma1	1
Chiesi-Phönix	Asche Basis® cream	91425A	1
Chiesi-Phönix	Asche Basis® cream	91430A	2
Chinesi / Sanacorp	Asche Basis® cream	13009A	1
Chinesi / Sanacorp	Asche Basis® cream	14017A	1
Chisei	Asche Basis® cream	72382A	1
Chisesi/Noweda	Asche Basis® cream	53331A	1

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Supplier	Substance	Batch	Spectra
Chisesi/Noweda	Asche Basis® cream	61338A	1
Chisesi/Noweda	Asche Basis® cream	71367A	1
Chisesi	Asche Basis® cream	52310A	1
Chisie/ Jenne	Asche Basis® cream	4004A	1
Chisie/ Jenne	Asche Basis® cream	91431A	1
Chisie/VDL	Asche Basis® cream	84417A	2
Dermapharm	Excipial® U Lipolotio	169010	1
Dermapharm	Excipial® U Lipolotio	311839	1
Dermapharm	Excipial® U Lipolotio	319748	1
Dermasence/Anzag	Dermatest base ointment	260820	2
Dermasence/Gehe	Dermatest base ointment	280821	2
Dermasense/ Sanacorp	Dermatest base ointment	40622	1
Devesa	Asche Basis® lotion	63078A	1
Dr. Wolff	Abitima® clinic face cream	15726	1
Dr.Wolff	Asche Basis® cream		1
Ebert & Jacobi	Asche Basis® lotion	73088A	1
Ebert und Jacobi	Asche Basis® cream	82405A	1
Eucerinum/Phönnix	Eucerinum W/O basis	94930108	1
eucerinum	Eucerinum W/O basis	41830108WA	1
Euro OTC	Fabitop® base cream	1016021	1
Euro OTC	Hans Karrer Lipolotion Micro...	16010	1
Euro OTC	Asche Basis® cream	3229A	1
Euro OTC	Asche Basis® cream	61337A	2
Euro OTC	Asche Basis® cream	74391A	1
Euro OTC	Asche Basis® cream	82405A	1
Euro OTC	Dermatop® base cream	8F077A	1
Euro OTC	Neribas® cream	YY02805	1
Euro/ Phönix	Excipial® U Lipolotio	4417A-03749	1
Fa. Chiesi/Gehe	Asche Basis® cream	2456A	1
Fa. Chiesi/Gehe	Asche Basis® lotion	92100A	2
Fa. Chiesi/Gehe	Asche Basis® lotion	94106A	1
Fa. Chiesi/NOweda	Asche Basis® cream	1454A	1
Fa. Chiesi/NOweda	Asche Basis® cream	2457A	1
Fa. Chiesi/NOweda	Asche Basis® cream	2459A	1
Fa. Chiesi/Noweda	Asche Basis® lotion	91097A	3
Fa. Chiesi/NOweda	Asche Basis® cream	92439A	1
Fa. Chiesi/NOweda	Asche Basis® cream	93444A	1
Fa.Chiesi/Gehe	Asche Basis® cream	91428A	1
Fa.Chiesi/Gehe	Asche Basis® cream	91430A	1
Fa.Chiesi/Noweda	Asche Basis® lotion	94104A	1
Fa.Chiesi/Noweda	Asche Basis® lotion	94105A	1
Fa.Gehe	Excipial® hydro cream	20160727Ma3	1
Fa.Gehe	Asche Basis® cream	20160727Ma4	1
Fa.Gehe	Asche Basis® lotion	20160727Ma5	1
Fagron	Abitima® clinic body cream	110517	2
Fagron	Abitima® clinic face cream	150204	1
Fagron	Base cream Taoasis	20B10-T13-075420	1
Fagron	Abitima® clinic body cream	241118	1
Fagron	Abitima® clinic body cream	251118	2
Fagron	Asche Basis® cream	63353A	1
Fagron	Excipial® U Lipolotio	N168	2
Fagron	Excipial® U Lipolotio	T123	1
Fagron	Excipial® U Lipolotio	V081	1
Fiebig/Chiesi GmbH	Asche Basis® cream	73388A	1
Fiebig/Chiesi GmbH	Asche Basis® cream	81404A	1
Fiebig/Chiesi	Asche Basis® lotion	71083A	1
Fiebig/Chiesi	Asche Basis® lotion	71084A	3
Fiebig/Chiesi	Asche Basis® lotion	73087A	2
Fiebig/Chiesi	Asche Basis® lotion	82092A	2
Fiebig/Chiesi	Asche Basis® lotion	84095A	1

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Supplier	Substance	Batch	Spectra
Fiebig/DR.Wolf	Excipial® U Lipolotio	V028	1
Fiebig/Galderma	Excipial® U Lipolotio	V101	1
Fiebig	Asche Basis® cream	13011A	1
Fiebig	Eucerinum W/O basis	80330108WA	1
Fiebig	Asche Basis® cream	83413A	3
Fiebig	Asche Basis® cream	84420A	1
Fiebig	Asche Basis® cream	84421A	1
Fiebig	Asche Basis® lotion	91097A	1
Fiebig	Asche Basis® cream	91428A	2
Fiebig	Excipial® U Lipolotio	T061	2
Fischar	Excipial® U Lipolotio	LOTNO85	1
Fontapharm / Phönix	Fabitop® base cream	1016022	2
Fontapharm / Phönix	Fabitop® base cream	101603	5
Fontapharm / Phönix	Fabitop® base cream	520012	2
fontapharm AG	Fabitop® base cream	101601	1
Fontapharm AG	Fabitop® base cream	52002	2
Fontapharm/ Phoenix	Fabitop® base cream	520011	2
Fontapharm/Anzag	Fabitop® base cream	101601	1
Fontapharm/Gehe	Fabitop® base cream	GLWD4	1
Fontapharm/Gotha	Fabitop® base cream	520011	2
Fontapharm/Noweda (17.0…	Fabitop® base cream	520011	4
Fontapharm/Noweda	Fabitop® base cream	101601	1
Fontapharm/Noweda	Fabitop® base cream	GLWD3	1
Fontapharm/Phönix	Fabitop® base cream	101601	9
Fontapharm/Phönix	Fabitop® base cream	520011	3
Fontapharm/phönix	Fabitop® base cream	52002	1
Fontapharm/Phönix	Fabitop® base cream	GLWD2	1
Fontapharm/Phönix	Fabitop® base cream	GLWD5	1
Fontapharm/Sanacop	Fabitop® base cream	101601	4
Fontapharm	Fabitop® base cream	101601	1
Fontapharm	Fabitop® base cream	GLWD2	9
Fontapharm	Fabitop® base cream	GLWD2x2	1
Fontapharm	Fabitop® base cream	GLWD3	2
Fontapharm	Fabitop® base cream	GLWD5	1
Fontapharm	Fabitop® base cream	GLWW4	1
Fontapharma AG / Noweda	Fabitop® base cream	1016021	1
Galaderma/Krieger	Excipial® U Lipolotio	173469	1
Galaderma/Krieger	Asche Basis® cream	17370A	1
Galaderma/Krieger	Excipial® U Lipolotio	174756	1
Galaderma/Krieger	Excipial® U Lipolotio	303485	1
Galaderma/Krieger	Excipial® U Lipolotio	309994	1
Galaderma/Krieger	Excipial® U Lipolotio	318628	1
Galaderma/Krieger	Excipial® U Lipolotio	318718	1
Galaderma/Krieger	Excipial® U Lipolotio	LOT50249	1
Galaderma/Krieger	Excipial® U Lipolotio	LOT50842	1
Galaderma/Krieger	Excipial® U10 Lipolotio	T071	1
Galaderma/Krieger	Excipial® U Lipolotio	V011	1
Galaderma/Phönix	Excipial® U Lipolotio	LOTV152	1
Galaderma/Phönix	Excipial® U Lipolotio	V041	1
Galaderma	Excipial® U Lipolotio	R072	1
Galderma (Canada) Düsse…	Excipial® U Lipolotio	330444	1
Galderma (Spirig Pharma…	Excipial® U Lipolotio	R061	1
Galderma (Spirig Pharma…	Excipial® U Lipolotio	T057	1
Galderma / Noweda	Excipial® hydro cream	T052	1
Galderma / Noweda	Excipial® U Lipolotio	T115	1
Galderma / Noweda	Excipial® U Lipolotio	V152	1
Galderma / Alliance Hea…	Excipial® U Lipolotio	344109	1
Galderma / Fiebig	Excipial® U Lipolotio	327343	1
Galderma / Galderma	Excipial® U Lipolotio	R086	1
Galderma / Kehr	Excipial® U Lipolotio	R167	1

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Supplier	Substance	Batch	Spectra
Galderma / Kehr	Excipial® U Lipolotio	R171	1
Galderma / Kehr	Excipial® U Lipolotio	T029	2
Galderma / Noweda EK 5,60	Excipial® lipo cream	1769014	1
Galderma / Noweda	Excipial® U Lipolotio	T073/170522EUL	1
Galderma / Phoenix	Excipial® U Lipolotio	357791	2
Galderma / Phönix	Excipial® U Lipolotio	173041	1
Galderma / Phönix	Excipial® U Lipolotio	319748	1
Galderma / Phönix	Excipial® U Lipolotio	354830	2
Galderma /	Excipial® hydro cream	P28013-0	1
Galderma /AHD	Excipial® U Lipolotio	169853	1
Galderma /AHD	Excipial® lipo cream	50567	3
Galderma /AHD	Excipial® lipo cream	8769004	2
Galderma /AllianceHC	Lipoderm® lotion	T043	2
Galderma /Ebert	Excipial® U Lipolotio	T156	1
Galderma /Fiebig	Excipial® U Lipolotio	170615	2
Galderma /Noweda	Excipial® hydro cream	1767002	1
Galderma /Phönix	Excipial® hydro cream	LOTT052	2
Galderma International ...	Excipial® lipo cream	1769017	1
Galderma International ...	Excipial® U Lipolotio	334288	2
Galderma International ...	Excipial® U Lipolotio	344636	1
Galderma International ...	Excipial® hydro cream	767004	1
Galderma International ...	Excipial® lipo cream	769002	1
Galderma International/...	Excipial® U Lipolotio	167638	1
Galderma International/...	Excipial® U Lipolotio	171711	1
Galderma International/...	Excipial® U Lipolotio	173041	1
Galderma International/...	Excipial® U Lipolotio	314142	1
Galderma International/...	Excipial® U Lipolotio	319748	1
Galderma International/...	Excipial® U Lipolotio	50876	1
Galderma International/...	Excipial® lipo cream	769002	1
Galderma International/...	Excipial® lipo cream	769005	1
Galderma International/...	Excipial® hydro cream	9767002	1
Galderma International/...	Excipial® U Lipolotio	V121	1
Galderma Labor.	Excipial® U Lipolotio	169010	1
Galderma Labor.	Excipial® U Lipolotio	169110	1
Galderma Labor.	Excipial® U Lipolotio	310709	2
Galderma Labor.	Excipial® U Lipolotio	312811	1
Galderma Laboratorium G...	Excipial® hydro cream	50564	1
Galderma Laboratorium G...	Excipial® hydro cream	9767005	1
Galderma Laboratorium G...	Excipial® hydro cream	9767006	1
Galderma über Phönix	Excipial® U Lipolotio	319422	1
Galderma über Phönix	Excipial® U Lipolotio	342479	1
Galderma, Sanacorp	Excipial® U Lipolotio	LOTS042	1
Galderma/ Alliance	Excipial® U Lipolotio	T115	1
Galderma/ Fiebig	Excipial® U Lipolotio	830071/17	1
Galderma/ Fiebig	Excipial® lipo cream	LOTV111	1
Galderma/ Galderma	Excipial® U Lipolotio	327343	1
Galderma/ Galderma	Excipial® U Lipolotio	332540	1
Galderma/ Gehe	Excipial® lipo cream	1769003	4
Galderma/ Gehe	Excipial® U Lipolotio	323922	4
Galderma/ Gehe	Excipial® lipo cream	769002	1
Galderma/ Gehe	Excipial® hydro cream	V051	1
Galderma/ Jenne	Excipial® lipo cream	1769001	1
Galderma/ Noweda	Excipial® U Lipolotio	169110	1
Galderma/ Noweda	Excipial® U Lipolotio	174756	1
Galderma/ Noweda	Excipial® U Lipolotio	312417	1
Galderma/ Noweda	Excipial® U Lipolotio	319844	1
Galderma/ Noweda	Excipial® U Lipolotio	326881	1
Galderma/ Noweda	Excipial® U Lipolotio	50876	2
Galderma/ Noweda	Excipial® U Lipolotio	LOT50450	1
Galderma/ Noweda	Excipial® hydro cream	LOT50782	1

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Supplier	Substance	Batch	Spectra
Galderma/ Noweda	Excipial® lipo cream	s023	6
Galderma/ Noweda	Excipial® lipo cream	S031	9
Galderma/ Noweda	Excipial® lipo cream	T021	5
Galderma/ Noweda	Excipial® lipo cream	t022	5
Galderma/ Noweda	Excipial® lipo cream	T022	4
Galderma/ Noweda	Excipial® U Lipolotio	T072	1
Galderma/ NOWEDA	Excipial® U Lipolotio	V082	1
Galderma/ Phönix	Excipial® U Lipolotio	330444	1
Galderma/ Phönix	Excipial® lipo cream	9769004	1
Galderma/ Phönix	Excipial® lipo cream	9769030	2
Galderma/ Sana	Excipial® hydro cream	S024	1
Galderma/ Sana	Excipial® hydro cream	S025	1
Galderma/ Sanacorp	Excipial® lipo cream	50567	1
Galderma/ Sanacorp	Excipial® lipo cream	8769004	1
Galderma/ Sanacorp	Excipial® lipo cream	LOT50567	1
Galderma/	Excipial® U Lipolotio	319921	1
Galderma/	Excipial® lipo cream	9769004	1
Galderma/	Excipial® hydro cream	S012	1
Galderma/	Excipial® hydro cream	V011	1
Galderma/	Excipial® hydro cream	VO11	1
Galderma/AEP	Excipial® U Lipolotio	314603	1
Galderma/AEP	Excipial® U Lipolotio	V165	1
Galderma/AHCA	Excipial® lipo cream	9769004	1
Galderma/AHCA	Excipial® U10 Lipolotio	LOT50604	1
Galderma/AHD	Excipial® U Lipolotio	323580	1
Galderma/AHD	Excipial® U Lipolotio	344636	1
Galderma/AHD	Excipial® hydro cream	9767001	1
Galderma/AHD	Excipial® hydro cream	9767005	1
Galderma/AHD	Excipial® hydro cream	9767006	1
Galderma/Alliance Heal…	Excipial® U Lipolotio	330444	1
Galderma/Alliance Healt…	Excipial® hydro cream	S025	1
Galderma/Alliance Healt…	Excipial® U Lipolotio	T121	1
Galderma/Alliance	Excipial® U Lipolotio	305489	1
Galderma/Alliance	Excipial® U10 Lipolotio	323868	1
Galderma/Alliance	Lipoderm® lotion	50316	2
Galderma/Alliance	Excipial® lipo cream	769002	1
Galderma/Alliance	Excipial® lipo cream	769013	2
Galderma/Alliance	Lipoderm® lotion	LOTV012	2
Galderma/Alliance	Excipial® U Lipolotio	S135	1
Galderma/Alliance	Excipial® U10 Lipolotio	T042	1
Galderma/Alliance	Excipial® hydro cream	T052	1
Galderma/Alliance	Excipial® lipo cream	T061	1
Galderma/Alliance	Excipial® U Lipolotio	T122	1
Galderma/Alliance	Excipial® U Lipolotio	V041	1
Galderma/Alliance	Excipial® lipo cream	V091	2
Galderma/Alliance	Excipial® lipo cream	V112	1
Galderma/AllianceHC	Lipoderm® lotion	T011	2
Galderma/anzag	Excipial® U Lipolotio	363069	2
Galderma/Anzag	Excipial® U Lipolotio	R183	1
Galderma/Anzag	Excipial® lipo cream	S011	1
Galderma/Anzag	Excipial® U Lipolotio	S206	1
Galderma/Direkt	Excipial® U Lipolotio	319748	1
Galderma/Ebert	Excipial® U Lipolotio	V082	1
Galderma/Ebert	Excipial® hydro cream	V041	1
Galderma/Fiebig	Excipial® hydro cream	1767001	1
Galderma/Fiebig	Excipial® U Lipolotio	319844	2
Galderma/Fiebig	Excipial® U Lipolotio	338630	1
Galderma/Fiebig	Excipial® U Lipolotio	V062	1
galderma/G	Excipial® U Lipolotio	LOTS202	1
Galderma/Galderma	Excipial® U Lipolotio	174960	1

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Supplier	Substance	Batch	Spectra
Galderma/Galderma	Excipial® U10 Lipolotio	308310	1
Galderma/Galderma	Excipial® lipo cream	50567	1
Galderma/Galderma	Excipial® U Lipolotio	50852	1
Galderma/Galderma	Excipial® lipo cream	8769004	1
Galderma/Galderma	Excipial® lipo cream	R042	9
Galderma/Galderma	Excipial® lipo cream	ro26	1
Galderma/Galderma	Excipial® lipo cream	RO26	1
Galderma/Galderma	Excipial® U Lipolotio	s017	1
Galderma/Galderma	Excipial® U Lipolotio	S017	1
Galderma/Galderma	Excipial® lipo cream	S023	8
Galderma/Galderma	Excipial® hydro cream	S024	2
Galderma/Galderma	Excipial® hydro cream	S054	1
Galderma/Galderma	Excipial® U Lipolotio	S142	1
Galderma/Galderma	Excipial® hydro cream	so25	1
Galderma/Galderma	Excipial® lipo cream	T021	8
Galderma/Galderma	Excipial® hydro cream	V042	1
Galderma/Galderma	Excipial® hydro cream	V051	1
Galderma/Galderma	Excipial® lipo cream	V121	1
Galderma/Gehe	Excipial® U Lipolotio	169831	1
Galderma/Gehe	Excipial® U Lipolotio	171710	1
Galderma/Gehe	Excipial® lipo cream	1769001	1
Galderma/Gehe	Excipial® U Lipolotio	312417	1
Galderma/Gehe	Excipial® U Lipolotio	312811	2
Galderma/Gehe	Excipial® U10 Lipolotio	329100	1
Galderma/Gehe	Excipial® U Lipolotio	332540	1
Galderma/Gehe	Excipial® U Lipolotio	335695	1
Galderma/Gehe	Excipial® U Lipolotio	346461	1
Galderma/Gehe	Excipial® U Lipolotio	352411	2
Galderma/Gehe	Excipial® U Lipolotio	357791	1
Galderma/Gehe	Excipial® U Lipolotio	368866	1
Galderma/Gehe	Excipial® U Lipolotio	50450	1
Galderma/Gehe	Excipial® U Lipolotio	50691	1
Galderma/Gehe	Excipial® U Lipolotio	50842	1
Galderma/Gehe	Excipial® lipo cream	50849	1
Galderma/Gehe	Excipial® hydro cream	767004	1
Galderma/Gehe	Excipial® lipo cream	769002	4
Galderma/Gehe	Excipial® hydro cream	8767001	1
Galderma/Gehe	Excipial® hydro cream	9757001	1
Galderma/Gehe	Excipial® hydro cream	9767001	2
Galderma/Gehe	Excipial® hydro cream	9767002	1
Galderma/Gehe	Excipial® U Lipolotio	LOT50450	1
Galderma/Gehe	Excipial® hydro cream	R031	1
Galderma/Gehe	Excipial® lipo cream	R042	2
Galderma/Gehe	Excipial® U Lipolotio	R189	1
Galderma/Gehe	Excipial® U Lipolotio	S139	1
Galderma/Gehe	Excipial® U Lipolotio	T061	1
Galderma/Gehe	Excipial® U Lipolotio	T066	1
Galderma/Gehe	Excipial® U Lipolotio	T156	2
Galderma/Gehe	Excipial® hydro cream	V042	1
Galderma/Gehe	Excipial® hydro cream	V071	1
Galderma/Gehe	Excipial® hydro cream	V072	2
Galderma/Gehe	Excipial® lipo cream	V091	1
Galderma/Gehe	Excipial® U Lipolotio	V108	1
Galderma/Graf-Eberhard-...	Excipial® U Lipolotio	174966	1
Galderma/Graf-Eberhard-...	Excipial® U Lipolotio	310709	1
Galderma/Jenne	Excipial® hydro cream	1767003	1
Galderma/Jenne	Excipial® U Lipolotio	326881	1
Galderma/Jenne	Excipial® U Lipolotio	355167	1
Galderma/Kehr	Excipial® lipo cream	1769017	1
Galderma/Kehr	Excipial® U Lipolotio	320973	1

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Supplier	Substance	Batch	Spectra
Galderma/Kehr	Lipoderm® lotion	S021	2
Galderma/Kehr	Excipial® U Lipolotio	S071	1
Galderma/Kehr	Excipial® U Lipolotio	S203	1
Galderma/Krieger	Excipial® U10 Lipolotio	308310	1
Galderma/Krieger	Excipial® U10 Lipolotio	50581	3
Galderma/Krieger	Excipial® U Lipolotio	50689	3
Galderma/Noweda (04.08....	Excipial® hydro cream	767004	1
Galderma/Noweda	Excipial® U Lipolotio	170316EL/LOTT073	1
Galderma/Noweda	Excipial® hydro cream	170420EH/LOTT012	1
Galderma/Noweda	Excipial® lipo cream	170420EL/LOTT021	1
Galderma/Noweda	Excipial® U Lipolotio	170420EUL/LOTS204	1
Galderma/Noweda	Excipial® U Lipolotio	170518EUL/LOTT073	1
Galderma/Noweda	Excipial® hydro cream	170706EH/LOTT091	1
Galderma/Noweda	Excipial® U Lipolotio	170906EL/T072	1
Galderma/Noweda	Excipial® lipo cream	171819E/LOTT021	1
Galderma/Noweda	Excipial® lipo cream	1769003	2
Galderma/Noweda	Excipial® lipo cream	1769017	3
Galderma/Noweda	Excipial® lipo cream	180208L/LOTV091	1
Galderma/Noweda	Excipial® hydro cream	180319EH/LOTV051	1
Galderma/Noweda	Excipial® U Lipolotio	314142	1
Galderma/Noweda	Excipial® U Lipolotio	319422	1
Galderma/Noweda	Excipial® U Lipolotio	319844	1
Galderma/Noweda	Excipial® U Lipolotio	320973	1
Galderma/Noweda	Excipial® U Lipolotio	323580	1
Galderma/Noweda	Excipial® U Lipolotio	324788	1
Galderma/Noweda	Excipial® U Lipolotio	326331	1
Galderma/Noweda	Excipial® U Lipolotio	330444	4
Galderma/Noweda	Excipial® U Lipolotio	332540	1
Galderma/Noweda	Excipial® U Lipolotio	342479	1
Galderma/Noweda	Excipial® U Lipolotio	344636	1
Galderma/Noweda	Excipial® U Lipolotio	354830	1
Galderma/Noweda	Excipial® U Lipolotio	363075	1
Galderma/Noweda	Excipial® hydro cream	50564	1
Galderma/Noweda	Excipial® lipo cream	50567	1
Galderma/Noweda	Excipial® U Lipolotio	50689	2
Galderma/Noweda	Excipial® hydro cream	50782	1
Galderma/Noweda	Excipial® U Lipolotio	50842	2
Galderma/Noweda	Excipial® lipo cream	50849	2
Galderma/Noweda	Excipial® hydro cream	767001	1
Galderma/Noweda	Excipial® lipo cream	769013	1
Galderma/Noweda	Excipial® lipo cream	9769004	1
Galderma/Noweda	Excipial® lipo cream	9769030	1
Galderma/Noweda	Excipial® lipo cream	R011	1
Galderma/Noweda	Excipial® lipo cream	R026	2
Galderma/Noweda	Excipial® hydro cream	S054	2
Galderma/Noweda	Excipial® lipo cream	T021	1
Galderma/Noweda	Excipial® U Lipolotio	V011	1
Galderma/Noweda	Excipial® U Lipolotio	V041	1
Galderma/Noweda	Excipial® hydro cream	V042	1
Galderma/Noweda	Excipial® hydro cream	V051	2
Galderma/Noweda	Excipial® U Lipolotio	V082	1
Galderma/Noweda	Excipial® U Lipolotio	V141	1
Galderma/Noweda	Excipial® U Lipolotio	V143	1
Galderma/phoen	Excipial® U Lipolotio	V166	1
Galderma/Phoenix(17.08....	Excipial® hydro cream	1767003A	1
Galderma/Phoenix(30.06....	Excipial® U Lipolotio	355167	2
Galderma/phoenix	Excipial® U Lipolotio	169010	1
Galderma/phoenix	Excipial® U Lipolotio	169847	1
Galderma/phoenix	Excipial® U Lipolotio	171711	3
Galderma/Phoenix	Excipial® U Lipolotio	173469	1

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Supplier	Substance	Batch	Spectra
Galderma/Phoenix	Excipial® U Lipolotio	174966	1
Galderma/Phoenix	Excipial® U Lipolotio	175042	2
Galderma/Phoenix	Excipial® hydro cream	1767002	1
Galderma/Phoenix	Excipial® U10 Lipolotio	308310	2
Galderma/Phoenix	Excipial® U Lipolotio	308637	2
Galderma/phoenix	Excipial® U Lipolotio	310709	5
Galderma/Phoenix	Excipial® U Lipolotio	312417	2
Galderma/Phoenix	Excipial® U Lipolotio	314603	2
Galderma/Phoenix	Excipial® U Lipolotio	319422	4
Galderma/Phoenix	Excipial® U Lipolotio	319748	1
Galderma/Phoenix	Excipial® U Lipolotio	355167	1
Galderma/Phoenix	Excipial® U Lipolotio	3717E-03749	1
Galderma/Phoenix	Excipial® hydro cream	50235	1
Galderma/Phoenix	Excipial® U Lipolotio	50450	1
Galderma/Phoenix	Excipial® hydro cream	50515	2
Galderma/Phoenix	Excipial® hydro cream	50634	1
Galderma/Phoenix	Excipial® hydro cream	50782	4
Galderma/Phöenix	Lipoderm® lotion	50932	1
Galderma/Phoenix	Excipial® hydro cream	767001	1
Galderma/Phoenix	Excipial® lipo cream	8769004	1
Galderma/Phoenix	Excipial® hydro cream	9767001	3
Galderma/Phoenix	Excipial® hydro cream	9767002	1
Galderma/Phoenix	Excipial® hydro cream	9767005	4
Galderma/Phoenix	Excipial® U Lipolotio	LOTT085	1
Galderma/Phoenix	Lipoderm® lotion	S041	1
Galderma/Phoenix	Excipial® hydro cream	V031	1
Galderma/Phoenix	Excipial® U Lipolotio	V041	1
Galderma/Phoenix	Excipial® U Lipolotio	V061	1
Galderma/Phoenix	Excipial® hydro cream	V071	1
Galderma/Phoenix	Excipial® U Lipolotio	VO11	1
Galderma/Phönic	Excipial® hydro cream	VO61	1
Galderma/Phönix WE: 03...	Excipial® lipo cream	LOTV012	1
Galderma/Phönix	Excipial® U Lipolotio	170195	1
Galderma/Phönix	Excipial® U Lipolotio	170615	4
Galderma/Phönix	Excipial® U Lipolotio	173469	4
Galderma/Phönix	Excipial® U10 Lipolotio	174116	1
Galderma/Phönix	Excipial® U Lipolotio	174756	1
Galderma/Phönix	Hans Karrer Lipolotion Micro...	20005	1
Galderma/Phönix	Excipial® U Lipolotio	309994	1
Galderma/Phönix	Excipial® U Lipolotio	311839	1
Galderma/Phönix	Excipial® U Lipolotio	314603	1
Galderma/Phönix	Excipial® U Lipolotio	319748	2
Galderma/Phönix	Excipial® U Lipolotio	326881	2
Galderma/Phönix	Excipial® hydro cream	50235	1
Galderma/Phönix	Excipial® hydro cream	50515	1
Galderma/Phönix	Excipial® lipo cream	50567	6
Galderma/Phönix	Excipial® U Lipolotio	50569	1
Galderma/Phönix	Excipial® lipo cream	50627	1
GAlderma/Phönix	Excipial® lipo cream	50627	2
Galderma/Phönix	Excipial® hydro cream	50782	4
Galderma/Phönix	Excipial® U Lipolotio	50876	1
Galderma/Phönix	Excipial® lipo cream	8769004	1
Galderma/Phönix	Excipial® hydro cream	9767005	1
Galderma/Phönix	Excipial® lipo cream	9769004	3
Galderma/Phönix	Excipial® lipo cream	9769010	1
Galderma/Phönix	Excipial® lipo cream	9769011	6
Galderma/Phönix	Excipial® lipo cream	R026	2
Galderma/Phönix	Excipial® lipo cream	RO12	1
Galderma/Phönix	Excipial® lipo cream	RO42	1
Galderma/Phönix	Excipial® hydro cream	S013	1

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Supplier	Substance	Batch	Spectra
Galderma/Phönix	Excipial® lipo cream	S023	1
Galderma/Phönix	Excipial® lipo cream	S031	1
Galderma/Phönix	Excipial® hydro cream	S045	1
Galderma/Phönix	Excipial® lipo cream	S032	1
Galderma/Phönix	Excipial® lipo cream	T021	1
Galderma/Phönix	Lipoderm® lotion	T043	1
Galderma/Phönix	Excipial® hydro cream	T081	1
Galderma/phönix	Excipial® U Lipolotio	T091	2
Galderma/Phönix	Excipial® U Lipolotio	T116	1
Galderma/Phönix	Excipial® U Lipolotio	T149	1
Galderma/Phönix	Excipial® hydro cream	V011	2
Galderma/Phönix	Excipial® U Lipolotio	V035	1
Galderma/Phönix	Excipial® U Lipolotio	V041	2
Galderma/Phönix	Excipial® hydro cream	V052	1
Galderma/Phönix	Excipial® hydro cream	V071	1
Galderma/Phönix	Excipial® U Lipolotio	V136	1
Galderma/Phonix	Excipial® U Lipolotio	V157	1
Galderma/phönix	Excipial® U Lipolotio	V162	1
Galderma/Sanacorp	Excipial® U Lipolotio	167638	1
Galderma/Sanacorp	Excipial® U10 Lipolotio	169759	2
galderma/sanacorp	Excipial® lipo cream	1769001	1
Galderma/Sanacorp	Excipial® lipo cream	1769003	2
Galderma/Sanacorp	Excipial® lipo cream	1769014	2
Galderma/Sanacorp	Excipial® lipo cream	1769017	1
Galderma/Sanacorp	Excipial® U10 Lipolotio	308601	3
Galderma/Sanacorp	Excipial® U10 Lipolotio	308637	1
Galderma/Sanacorp	Excipial® U Lipolotio	309197	1
Galderma/sanacorp	Excipial® U Lipolotio	310709	1
Galderma/Sanacorp	Excipial® U Lipolotio	311839	2
Galderma/Sanacorp	Excipial® U Lipolotio	314142	1
Galderma/Sanacorp	Excipial® U Lipolotio	319351	1
Galderma/Sanacorp	Excipial® U Lipolotio	319748	1
Galderma/Sanacorp	Excipial® U10 Lipolotio	320154	1
Galderma/Sanacorp	Excipial® U10 Lipolotio	321879	1
Galderma/Sanacorp	Excipial® U10 Lipolotio	322729	1
Galderma/Sanacorp	Excipial® U10 Lipolotio	323868	1
Galderma/Sanacorp	Excipial® U Lipolotio	326881	1
Galderma/Sanacorp	Excipial® U Lipolotio	330444	1
Galderma/Sanacorp	Excipial® U Lipolotio	334288	1
Galderma/Sanacorp	Excipial® U Lipolotio	344636	1
Galderma/Sanacorp	Excipial® U10 Lipolotio	50679	1
Galderma/Sanacorp	Excipial® hydro cream	769013	1
Galderma/Sanacorp	Excipial® lipo cream	9769010	2
Galderma/Sanacorp	Excipial® lipo cream	9769030	7
Galderma/Sanacorp	Excipial® hydro cream	LOTV041	1
Galderma/Sanacorp	Excipial® U Lipolotio	V038	1
Galderma/Sanacorp	Excipial® U Lipolotio	V073	1
Galderma/Sanacorp	Excipial® U10 Lipolotio	V092	1
Galderma/Sanacorp	Excipial® U Lipolotio	V103	2
Galderma/Sanacorp	Excipial® U Lipolotio	V151	1
Galderma/Spirig Pharma AG	Excipial® U Lipolotio	LOTR187	1
Galderma/spirig	Excipial® U Lipolotio	S123	1
Galderma/Waldau Apotheke	Excipial® U Lipolotio	311839	2
Galderma/Würmi	Excipial® hydro cream	R031	1
Galderma/Würmtal Apotheke	Excipial® U Lipolotio	S132	2
Galderma/Würmtal-Apo.	Excipial® U10 Lipolotio	T053	1
Galderma/Würmtalapo	Excipial® lipo cream	R042	2
Galderma/Würmtal-APO	Excipial® hydro cream	S041	1
Galderma/Würmtal-Apotheke	Excipial® U Lipolotio	169010	1
Galderma/Würmtal-Apotheke	Excipial® U Lipolotio	50852	1

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Supplier	Substance	Batch	Spectra
Galderma/Würmtal-Apotheke	Excipial® U Lipolotio	R142	1
Galderma/Würmtal-Apotheke	Excipial® U Lipolotio	S071	4
Galderma/Würmtal-Apotheke	Excipial® U Lipolotio	S205	2
Galderma/Würmtal-Apotheke	Excipial® U Lipolotio	T149	1
Galderma/Würmtal-Apotheke	Excipial® U10 Lipolotio	V042	1
Galderma/Würmtal-Apotheke	Excipial® U Lipolotio	V142	1
Galderma	Excipial® U10 Lipolotio	15166	1
Galderma	Excipial® U Lipolotio	169005	1
Galderma	Excipial® U Lipolotio	169010	1
Galderma	Excipial® U Lipolotio	169110	4
Galderma	Excipial® U10 Lipolotio	169263	1
Galderma	Lipoderm® lotion	169310	4
Galderma	Excipial® U Lipolotio	169853	2
Galderma	Excipial® U Lipolotio	170195	1
Galderma	Excipial® U Lipolotio	170615	2
Galderma	Excipial® U Lipolotio	173469	2
Galderma	Excipial® U10 Lipolotio	174117	1
Galderma	Excipial® U Lipolotio	174756	1
Galderma	Excipial® lipo cream	1769001	1
Galderma	Excipial® lipo cream	1769014	1
Galderma	Excipial® U Lipolotio	270918A	1
Galderma	Excipial® U10 Lipolotio	304231	1
Galderma	Excipial® U Lipolotio	304310	1
Galderma	Excipial® U Lipolotio	305489	4
Galderma	Excipial® U Lipolotio	308637	3
Galderma	Excipial® U Lipolotio	310709	3
Galderma	Excipial® U Lipolotio	311839	2
Galderma	Excipial® U Lipolotio	312417	2
Galderma	Excipial® U Lipolotio	312811	3
Galderma	Excipial® U Lipolotio	314142	2
Galderma	Excipial® U10 Lipolotio	318218	1
Galderma	Excipial® U Lipolotio	318628	1
Galderma	Excipial® U Lipolotio	318718	2
Galderma	Excipial® U Lipolotio	319351	2
Galderma	Excipial® U Lipolotio	319422	1
Galderma	Excipial® U Lipolotio	319748	13
Galderma	Excipial® U Lipolotio	319921	4
Galderma	Excipial® U Lipolotio	320973	2
Galderma	Excipial® U10 Lipolotio	322729	1
Galderma	Excipial® U Lipolotio	323580	1
Galderma	Excipial® U Lipolotio	323922	4
Galderma	Excipial® U Lipolotio	324788	1
Galderma	Excipial® U Lipolotio	326881	4
Galderma	Excipial® U Lipolotio	327343	1
Galderma	Excipial® U Lipolotio	330444	2
Galderma	Excipial® U Lipolotio	332540	2
Galderma	Excipial® U Lipolotio	334288	2
Galderma	Excipial® U Lipolotio	335167	1
Galderma	Excipial® U Lipolotio	335695	6
Galderma	Excipial® U Lipolotio	338630	1
Galderma	Excipial® U Lipolotio	339852	4
Galderma	Excipial® U Lipolotio	342479	2
Galderma	Excipial® U Lipolotio	344109	3
Galderma	Excipial® U Lipolotio	344636	2
Galderma	Excipial® U Lipolotio	350885	3
Galderma	Excipial® U Lipolotio	351025	1
Galderma	Excipial® U Lipolotio	351894	1
Galderma	Excipial® U Lipolotio	352411	1
Galderma	Excipial® U Lipolotio	355168	1
Galderma	Excipial® U Lipolotio	357791	1

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Supplier	Substance	Batch	Spectra
Galderma	Excipial® U Lipolotio	50295	1
Galderma	Excipial® U Lipolotio	50346	1
Galderma	Excipial® U Lipolotio	50458	1
Galderma	Excipial® U Lipolotio	50459	1
Galderma	Excipial® hydro cream	50564	1
Galderma	Excipial® lipo cream	50567	1
Galderma	Excipial® hydro cream	50634	2
Galderma	Excipial® U Lipolotio	50688	1
Galderma	Excipial® U Lipolotio	50691	2
Galderma	Excipial® hydro cream	50782	3
Galderma	Excipial® U Lipolotio	50842	1
Galderma	Excipial® U Lipolotio	50852	7
Galderma	Excipial® U Lipolotio	50890	1
Galderma	Lipoderm® lotion	50932	1
Galderma	Excipial® lipo cream	8769004	1
Galderma	Excipial® hydro cream	9767005	1
Galderma	Excipial® hydro cream	9767006	1
Galderma	Excipial® lipo cream	9769004	1
Galderma	Excipial® lipo cream	9769005	1
Galderma	Excipial® lipo cream	9769010	1
Galderma	Excipial® lipo cream	9769030	1
galderma	Excipial® lipo cream	LOT50627	1
Galderma	Excipial® U10 Lipolotio	LOT50679	1
Galderma	Excipial® hydro cream	LOT50782	1
Galderma	Excipial® lipo cream	LOTS032	1
Galderma	Excipial® U Lipolotio	LOTS123	1
Galderma	Excipial® lipo cream	LOTV041	1
Galderma	Excipial® hydro cream	LOTV051	1
Galderma	Excipial® hydro cream	LOTV071	2
Galderma	Excipial® hydro cream	LOTV072	1
Galderma	Excipial® U Lipolotio	LOTV121	1
Galderma	Excipial® lipo cream	N061	2
galderma	Excipial® U Lipolotio	R024	1
Galderma	Excipial® lipo cream	R026	2
Galderma	Excipial® lipo cream	R035	2
Galderma	Excipial® lipo cream	R042	1
Galderma	Lipoderm® lotion	R044	2
Galderma	Excipial® U Lipolotio	R111	1
Galderma	Excipial® U Lipolotio	R115	1
Galderma	Excipial® U Lipolotio	R143	1
Galderma	Excipial® U Lipolotio	R167	2
Galderma	Excipial® U Lipolotio	R168	1
Galderma	Excipial® U Lipolotio	R171	2
Galderma	Excipial® U Lipolotio	R172	1
Galderma	Excipial® lipo cream	RO12	1
Galderma	Lipoderm® lotion	S021	1
Galderma	Excipial® hydro cream	S041	1
Galderma	Excipial® hydro cream	S054	1
Galderma	Excipial® U Lipolotio	S064	1
Galderma	Excipial® U Lipolotio	S065	1
Galderma	Excipial® U Lipolotio	S091	1
Galderma	Excipial® U Lipolotio	S137	1
Galderma	Excipial® U Lipolotio	S147	1
Galderma	Excipial® U Lipolotio	S148	1
Galderma	Lipoderm® lotion	T011	1
Galderma	Excipial® lipo cream	T021	2
Galderma	Excipial® hydro cream	T052	5
Galderma	Excipial® U Lipolotio	T056	1
Galderma	Excipial® lipo cream	T061	2
Galderma	Excipial® U Lipolotio	T062	1

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Supplier	Substance	Batch	Spectra
Galderma	Excipial® U Lipolotio	T125	2
Galderma	Excipial® U Lipolotio	V011	1
Galderma	Excipial® U Lipolotio	V037	1
Galderma	Excipial® lipo cream	v042	1
Galderma	Excipial® hydro cream	V051	2
Galderma	Excipial® U Lipolotio	V053	3
Galderma	Excipial® U10 Lipolotio	V061	1
Galderma	Excipial® lipo cream	V091	1
Galderma	Excipial® U10 Lipolotio	V096	1
Galderma	Excipial® U Lipolotio	V101	1
Galderma	Excipial® U Lipolotio	V139	2
Galderma	Excipial® U Lipolotio	V152	1
Galderma	Excipial® U Lipolotio	V153	2
Galderma	Excipial® U Lipolotio	V159	1
Galderma	Excipial® U Lipolotio	V165	1
Galderma-Spirig,Gehe 14…	Excipial® hydro cream	V061-20180830Ma11	1
Galderma-Spirig	Excipial® hydro cream	50235-E20190115Ma10	1
Galderma-Spirig	Excipial® hydro cream	To52-20171127Ma11	1
Galderma-Spirig	Excipial® hydro cream	V041-20180619Ma8	1
Galdermna/Anzag	Excipial® U Lipolotio	171710	1
Galderna/Sanacorp	Excipial® U Lipolotio	314603	2
Galderna/Sanacorp	Excipial® U Lipolotio	327343	2
Galderna/Sanacorp	Excipial® lipo cream	50849	1
Galderna/Sanacorp	Excipial® hydro cream	767001	3
Galderna/Sanacorp	Excipial® hydro cream	767003	1
Galderna/Sanacorp	Excipial® hydro cream	767004	1
Galderna/Sanacorp	Excipial® lipo cream	769002	1
Galderna/Sanacorp	Excipial® lipo cream	8769004	1
Gallderma / Phönix	Excipial® hydro cream	9767005	1
Galmeda Noweda	Excipial® lipo cream	180504EL/LOTV112	1
Gehe Chiesi	Asche Basis® lotion	53075A-20160615Ma5	1
Gehe,Galderma Spirig	Excipial® hydro cream	R031-20160615Ma7	1
Gehe/Beiersdorf	Eucerinum W/O basis	51630108WA	1
Gehe/Beiersdorf	Eucerinum W/O basis	94930108	1
Gehe/Chesie	Asche Basis® cream	52318A	2
Gehe/Chiesi	Asche Basis® cream	1452A	1
Gehe/Chiesi	Asche Basis® cream	1453A	1
gehe/Chiesi	Asche Basis® cream	2458A	1
Gehe/Chiesi	Asche Basis® cream	32233A	1
Gehe/Chiesi	Asche Basis® cream	3461A	1
gehe/Chiesi	Asche Basis® lotion	43066A	1
Gehe/Chiesi	Asche Basis® cream	51296A	1
Gehe/Chiesi	Asche Basis® cream	84418A	2
Gehe/Chiesi	Asche Basis® cream	92440A	1
Gehe/Chiesi	Asche Basis® lotion	93103A	1
GEHE/GALDERMA 25_11:16	Excipial® U Lipolotio	S147	1
Gehe/Galderma	Excipial® U Lipolotio	352411	1
Gehe/Galderma	Excipial® lipo cream	LOTS031	1
Gehe/Galderma	Excipial® U Lipolotio	LotV011	1
Gehe	Neuroderm® moisturising cream		1
GEHE	Abitima® clinic body cream	100116	2
Gehe	Asche Basis® cream	14014A	1
GEHE	Excipial® U Lipolotio	174966	1
GEHE	Excipial® U Lipolotio	174996	1
Gehe	Abitima® clinic body cream	180125	1
Gehe	Dermatest base ointment	270623	1
GEHE	Excipial® U Lipolotio	309197	2
GEHE	Excipial® U Lipolotio	312811	1
Gehe	Asche Basis® cream	32236A	1
Gehe	Eucerinum W/O basis	32930208WA	1

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Supplier	Substance	Batch	Spectra
GEHE	Abitima® clinic body cream	331017	2
Gehe	Asche Basis® cream	33244A	1
Gehe	Excipial® U Lipolotio	354348	1
GEHE	Excipial® U Lipolotio	50459	1
GEHE	Excipial® U Lipolotio	50688	1
GEHE	Excipial® U Lipolotio	50890	2
Gehe	Asche Basis® cream	52321A	1
Gehe	Asche Basis® cream	61334A	1
Gehe	Asche Basis® cream	64358A	2
Gehe	Asche Basis® cream	64360A	1
GEHE	Asche Basis® cream	73387A	2
GEHE	Asche Basis® cream	81399A	1
Gehe	Asche Basis® lotion	82082A	1
GEHE	Asche Basis® cream	82410A	1
Gehe	Fabitop® base cream	GRWW2	6
Gehe	Excipial® lipo cream	N061	1
Gehe	Excipial® U Lipolotio	S132	1
Gehe	Excipial® U Lipolotio	S143	1
Gehe	Excipial® U Lipolotio	V121	1
Gehe	Excipial® U Lipolotio	V152	1
Gehe20.10.15	Asche Basis® lotion	52070A	1
Gehe-Chiesi	Asche Basis® cream	52308A	1
Gehe-Spring	Excipial® U Lipolotio	LOTR167	1
Geibo, Galderma	Excipial® hydro cream	1767003	1
Geibo/ Beiersdorf	Eucerinum W/O basis	72630108WA	1
Geibo/ Beiersdorf	Eucerinum W/O basis	83730308WA	1
Geibo/Beiersdorf	Eucerinum W/O basis	83730208WA	1
Geibo/Beiersdorf	Eucerinum W/O basis	83730308WA	1
Gepepharm/VDL	Asche Basis® cream	81399A	1
Gladerma/Ebert	Excipial® hydro cream	VO72	1
GP GmbH/Spangro	Neribas® cream	Y018FF	1
GP Grenzach Produktions…	Neribas® cream	YY0203H	1
GPGrenzach Produktion/P…	Neribas® cream	YY01673	1
HÄLSA Pharma GmbH ; INF…	Neuroderm® moisturising cream		1
Hans Karre/ Pönix	Hans Karrer Lipolotion Micro…	20003	1
Hans Karrer / Anzag	Hans Karrer Lipolotion Micro…	16004	1
Hans Karrer GmbH/Krieger	Hans Karrer Lipolotion Micro…	LOT19009	1
Hans Karrer GmbH	Hans Karrer Lipolotion Micro…	19011	1
Hans Karrer GmbH	Hans Karrer Lipolotion Micro…	20007	1
Hans Karrer GmbH	Hans Karrer Lipolotion Micro…	20013	1
Hans Karrer GmbH	Hans Karrer Lipocream MicroS…	LOT20005	1
Hans Karrer/Alliance	Hans Karrer Lipolotion Micro…	17003	2
Hans Karrer/Alliance	Hans Karrer Lipolotion Micro…	17009	1
Hans Karrer/Gehe	Hans Karrer Lipolotion Micro…	17002	20
Hans Karrer/Phoe	Hans Karrer Lipolotion Micro…	17011	1
Hans Karrer/Phoe	Hans Karrer Lipolotion Micro…	LOT18005	1
Hans Karrer/Phoenix	Hans Karrer Lipolotion Micro…	18010	2
Hans Karrer	Hans Karrer Lipocream MicroS…	19001	1
hans karrer	Hans Karrer Lipocream MicroS…	19005	1
Hans Karrer	Hans Karrer Lipolotion Micro…	20003	1
Hans Karrer	Hans Karrer Lipolotion Micro…	20007	1
Hans Karrer	Hans Karrer Lipolotion Micro…	21019	1
HansKarrer/Phoenix	Hans Karrer Lipocream MicroS…	19004	1
HansKarrer/Phönix	Hans Karrer Lipolotion Micro…	19004	1
HansKarrer/Phönix	Hans Karrer Lipolotion Micro…	21009	1
HansKarrer/Sanacorp	Hans Karrer Lipolotion Micro…	19011	1
HansKarrer/Sanacorp	Hans Karrer Lipolotion Micro…	20007	1
HansKarrer/Sanacorp	Hans Karrer Lipolotion Micro…	LOT20007	1
hanskarrer	Hans Karrer Lipolotion Micro…	17005	1
hanskarrer	Hans Karrer Lipolotion Micro…	17007	2

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Supplier	Substance	Batch	Spectra
hanskarrer	Hans Karrer Lipolotion Micro…	19009	1
hanskarrer	Hans Karrer Lipolotion Micro…	LOT17005	1
Hedinger/Noweda	Lipoderm® lotion	169310	1
Hedinger/Noweda	Asche Basis® cream	82405A	1
Hedinger	Asche Basis® cream	74398A	1
Ichthyol/Phönix	Lipoderm® lotion	LOTT043	1
Ichthyol/Sanacorp	Asche Basis® cream	24221A	1
Ichthyol-Gesellschaft	Eucerinum W/O basis	80330108WA	1
Infecto Pharm	Neuroderm® moisturising cream		1
Infecto/Phönix	Neuroderm® moisturising cream		2
InfectoParm/Pönix	Neuroderm® moisturising cream		1
InfectoPharm /AEP	Neuroderm® moisturising cream		2
InfectoPharm/ AHD	Neuroderm® moisturising cream		1
Infectopharm/AHD	Neuroderm® moisturising cream		4
Infectopharm/Alliance	Neuroderm® moisturising cream		4
Infectopharm/Fiebig	Neuroderm® moisturising cream		1
Infectopharm/Gehe	Neuroderm® moisturising cream		3
Infectopharm/Gehe	Neuroderm® moisturising cream	S0315081	1
Infectopharm/Kehr	Neuroderm® moisturising cream		1
Infectopharm/noweda	Neuroderm® moisturising cream		1
Infectopharm/Noweda	Neuroderm® moisturising cream		5
InfectoPharm/Noweda	Neuroderm® moisturising cream		3
Infectopharm/Phoenix	Neuroderm® moisturising cream		2
Infectopharm/Phönix	Neuroderm® moisturising cream		9
infectopharm	Neuroderm® moisturising cream		1
Infectopharm	Neuroderm® moisturising cream		8
InfectoPharm	Neuroderm® moisturising cream		19
InfectoPharma/Alliance …	Neuroderm® moisturising cream		2
InfectoPharma/Noweda	Neuroderm® moisturising cream		1
Infetopharm	Neuroderm® moisturising cream		1
Insel	Asche Basis® cream	72378A	1
Intendis / Gehe	Neribas® cream	21076A	1
Intendis / Sanacorp	Neribas® cream	24105A	1
Intendis GmbH	Neribas® cream	24089A	1
Jena/Alliance	Neribas® cream	YY023J5	1
Jenapharm / Gehe	Neribas® cream	34104C	1
Jenapharm / Gehe	Neribas® cream	YY023J5	1
Jenapharm / Gehe	Neribas® cream	YY02L84	1
Jenapharm / Noweda	Neribas® cream	YY02H20	2
Jenapharm / Sanacorp	Neribas® cream	YY02804	1
Jenapharm /Noweda	Neribas® cream	YY00C34	1
Jenapharm/ G	Neribas® cream	YY01KK7	1
Jenapharm/ Noweda	Neribas® cream	YY00216	1
Jenapharm/ Noweda	Neribas® cream	YY01TCN	1
Jenapharm/ Phönix	Neribas® cream	YY023J5	1
Jenapharm/	Neribas® cream	YY005HT	2
Jenapharm/	Neribas® cream	YY01KK7	1
Jenapharm/Alliance	Neribas® cream	YY000C3	2
Jenapharm/Alliance	Neribas® cream	YY001HS	1
Jenapharm/Alliance	Neribas® cream	YY006LX	1
Jenapharm/Gehe	Neribas® cream	YY005HT	1
Jenapharm/Gehe	Neribas® cream	YY006KY	1
Jenapharm/Gehe	Neribas® cream	YY01KK7	1
Jenapharm/gehe	Neribas® cream	yy02805	1
Jenapharm/Krieger	Neribas® cream	YY02805	1
Jenapharm/Krieger	Neribas® cream	YY02H20	1
Jenapharm/Noweda	Neribas® cream	YY00C35	2
Jenapharm/Noweda	Neribas® cream	YY00XEF	2
Jenapharm/Noweda	Neribas® cream	YY014NJ	2
Jenapharm/Noweda	Neribas® cream	YY01CXP	2

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Supplier	Substance	Batch	Spectra
Jenapharm/Phoenix	Neribas® cream	YY023J5	1
Jenapharm/Phoenix	Neribas® cream	YY02L84	1
Jenapharm/Phokd	Neribas® cream	YY0203H	2
Jenapharm/Phönx	Neribas® cream	YY02H20	1
Jenapharm/Sanacorp	Neribas® cream	YY02L84	1
Jenapharm	Neribas® cream	33100C	1
Jenapharm	Neribas® cream	YY01K94	1
Jenapharm	Neribas® cream	YY0203H	1
Jenapharm	Neribas® cream	YY0277H	1
Jenapharm	Neribas® cream	YY02805	3
Jenapharm	Neribas® cream	YY02H20	1
jenne artesan	Fabitop® base cream	GLWWW5	1
Jenne	Fabitop® base cream	GWWL1	1
Jenne	Excipial® hydro cream	S041	1
Jenne	Lipoderm® lotion	T011	1
Karo Pharm,Noweda	Neribas® cream	YY04P2E	1
Karo Pharm,Noweda	Neribas® cream	YY052E1	2
Karo Pharma / Gehe	Neribas® cream	22A87/75	1
Karo Pharma AB	Neribas® cream	YY04FEJ	1
Karo Pharma	Neribas® cream	YY04EYL	2
KARo Pharma	Neribas® cream	YY04EYL	1
Karo Pharma	Neribas® cream	YY04F1K	1
Karo/Jenne	Neribas® cream	YY04FEJ	1
Karo/Jenne	Neribas® cream	YY04FEK	2
Karo/Jenne	Neribas® cream	YY04FEL	1
Karo/Jenne	Neribas® cream	YY04P2E	2
Karo/Jenne	Neribas® cream	YY052E1	10
Karo/Jenne	Neribas® cream	YY052E2	3
Karopharm/Krieger	Neribas® cream	YY0431K	1
KaroPharma/Noweda	Neribas® cream	YY052E2	1
KARRER/ E	Hans Karrer Lipolotion Micro…	LOT17002	1
Kehr/Galderma	Excipial® U Lipolotio	T029	1
Kehr	Asche Basis® cream	72376A	1
Kehr	Asche Basis® lotion	73085A	1
Kirchstrasse	Hans Karrer Lipocream MicroS…	17001	1
Klindwort Apotheke Rath…	Dermatop® base cream	8F075A	1
KOKO direkt	DMS® base cream classic	L036L20	2
KOKO GmbH & Co KG	DMS® base cream classic	L036118	2
KOKO GmbH & Co KG	DMS® base cream classic	L036I18	2
KOKO GmbH & Co KG	DMS® base cream classic	L036l18	1
KOKO GmbH & Co KG	DMS® base cream classic	L062H18	6
KOKO GmbH & Co. KG	DMS® base cream high classic…	L018D16	1
KOKO GmbH & Co. KG	DMS® base cream high classic	L054B16	1
koko GmbH EK: EUR 38,30 /…	DMS® base cream classic	L008F17	1
Koko GmBH&Co KG	DMS® base cream classic	L038J16	1
KoKo GmbH&Co.KG	DMS® base cream high classic…	L013K16	3
KoKo GmbH&Co.KG	DMS® base cream high classic…	L016D17	3
KoKo GmbH&Co.KG	DMS® base cream high classic…	L027T19	1
KoKo GmbH&Co.KG	DMS® base cream high classic…	L030A18	2
KoKo GmbH&Co.KG	DMS® base cream high classic…	L030G18	1
KoKo GmbH&Co.KG	DMS® base cream high classic…	L035K17	1
KOKO GmbH&Co.KG	DMS® base cream classic	L075G19	1
KoKo GmbH&Co.KG	DMS® base cream high classic…	L030G18	2
KoKo GmbH&Co.KG	DMS® base cream high classic…	L034C18	1
KoKo GmbH/KoKo Gmbh	DMS® base cream classic		1
KoKo GmbH/KoKo Gmbh	DMS® base cream classic	11090E19	1
KOko GmbH	DMS® base cream classic	801010	1
KOKO Gmbh	DMS® base cream high classic	L002B19	5
KOKO GmbH	DMS® base cream classic	L003E16	1
KOKO Gmbh	DMS® base cream high classic	L004K18	4

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Supplier	Substance	Batch	Spectra
KOKO GmbH	DMS® base cream classic	L005A14	1
KOKO Gmbh	DMS® base cream high classic	L008K17	5
KOKO Gmbh	DMS® base cream high classic	L010E17	10
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	L019H17	1
KOKO Gmbh	DMS® base cream high classic	L019H17	5
Koko GmbH	DMS® base cream high classic…	L028A20	2
KOKO Gmbh	DMS® base cream high classic	l028c18	5
KOKO GmbH	DMS® base cream high classic	L030L16	3
Koko GmbH	DMS® base cream high classic	L031A14	1
Koko Gmbh	DMS® base cream high classic	L031D18	1
Koko Gmbh	DMS® base cream high classic	L033J17	3
Koko Gmbh	DMS® base cream high classic…	L035F17	1
KOKO Gmbh	DMS® base cream high classic	L042E18	5
KOKO Gmbh	DMS® base cream high classic	L050I18	5
Koko GmbH	DMS® base cream high classic	L050J18	2
KOKO Gmbh	DMS® base cream high classic	l053f18	3
Koko GmbH	DMS® base cream high classic…	L063H20	2
Koko GmbH	DMS® base cream high classic…	L072E19	1
KOKO Gmbh	DMS® base cream high classic	LO12G19	3
KOKO Gmbh	DMS® base cream high classic	LO34F21	4
KOKO Gmbh	DMS® base cream high classic	LO35L19	2
KOKO Gmbh	DMS® base cream high classic	lo74s19	2
Koko	DMS® base cream high classic…	L009F21	2
KoKo	DMS® base cream high classic…	L014C16	1
KOKO	DMS® base cream classic	L022S19	3
KOKO	DMS® base cream classic	L026A20	1
KOKO	DMS® base cream high classic	L031A14	1
Koko	DMS® base cream high classic	L034F21	1
KoKo	DMS® base cream high classic	L035L19	1
KOKO	DMS® base cream high classic…	L037B21	1
KOKO	DMS® base cream high classic	L045G21	2
KOKO	DMS® base cream high classic	L048L19	3
KOKO	DMS® base cream high classic	L057S20	1
KOKO	DMS® base cream high classic…	L063A21	1
KOKO	DMS® base cream high classic	L066A22	1
KOKO	DMS® base cream classic	L079E21	1
KOKO	DMS® base cream high classic	L079K20	2
KOKO	DMS® base cream high classic	L081F22	1
Koko	DMS® base cream high classic…	L083S21	3
KOKO	DMS® base cream high classic…	L089G21	3
Kremer	Asche Basis® cream	71367A	3
Krieger	Neribas® cream	3388	1
krieger	Asche Basis® cream	92436A	1
Lamotte / Gehe	Asche Basis® cream	34247A	1
Leo Pharma/Gehe	Neribas® cream	YY043TY	1
Leo Pharma/Krieger	Neribas® cream	YY0431J	1
LEO Pharma/Phönix	Neribas® cream	YY0431K	1
LEO Pharma/Phönix	Neribas® cream	YY04EYL	1
Leo Pharma/Sanacorp	Neribas® cream	YY02H20	1
Leo Pharma	Neribas® cream	yy0431ik	4
Leo Pharma	Neribas® cream	yy0431j	1
Leo Pharma	Neribas® cream	YY0431K	1
Leo Pharma	Neribas® cream	yy04EYL	1
Leo Pharma	Neribas® cream	YY04EYL	2
Leo Pharma	Neribas® cream	YY04FEJ	1
LEO/Jenne	Neribas® cream	YY043TY	1
LEO/Jenne	Neribas® cream	YY04EYL	3
Leopharm	Neribas® cream	YY02TTH	1

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Supplier	Substance	Batch	Spectra
Leyh GmbH	Dermatest base ointment	121217	1
Neribas/Jenne	Neribas® cream	YY0431J	1
Neribas/Jenne	Neribas® cream	YY0431K	3
Neribas	Neribas® cream	YY006KY	1
Neribas	Neribas® cream	YY02TTH	4
Nestle Skin Health	Excipial® lipo cream	311839	1
Nestle Skin /Sanacorp	Excipial® U Lipolotio	310709	1
Nestlé Skin Health/ Gehe	Excipial® U Lipolotio	323580	1
Nestle Skin Health/ Now...	Excipial® U Lipolotio	305489	1
Nestle Skin Health/ Now...	Excipial® U Lipolotio	314142	1
Nestlé Skin Health/Anzag	Excipial® U Lipolotio	174966	1
Nestle Skin Health/Gald...	Excipial® U Lipolotio	319844	1
Nestle Skin Health/Gehe	Excipial® U Lipolotio	174756	1
Nestle Skin Health/Kehr	Excipial® U Lipolotio	319844	1
Nestle Skin Health/Noweda	Excipial® U Lipolotio	305489	2
Nestle Skin Health/Phönix	Excipial® U Lipolotio	303485	1
Nestlé Skin Health/Phönix	Excipial® U Lipolotio	308637	1
Nestle Skin Health/Phönix	Excipial® U Lipolotio	311839	1
Nestle Skin Health/Sana...	Excipial® U Lipolotio	319344	1
Nestle Skin Health	Lipoderm® lotion	169310	1
Nestle Skin Health	Excipial® U Lipolotio	174756	1
Nestle skin health	Excipial® U Lipolotio	174966	1
Nestle Skin Health	Excipial® U Lipolotio	310709	1
Nestle Skin Health	Excipial® U Lipolotio	312417	1
Nestle Skin Health	Excipial® U10 Lipolotio	318209	2
Nestle Skin Health	Excipial® U Lipolotio	318718	1
Nestle Skin Health	Excipial® U Lipolotio	319748	1
Nestle Skin Health	Excipial® U Lipolotio	320973	1
Nestle Skin	Excipial® U Lipolotio	324788	1
NestlèSkinHealth/Phönix	Excipial® U Lipolotio	308637	1
NestlèSkinHealth/Phönix	Excipial® U Lipolotio	312417	1
NestlèSkinHealth/Phönix	Excipial® U Lipolotio	327343	1
Noweda Beiersdorf	Eucerinum W/O basis	83730308WA	1
Noweda/ Galderma	Excipial® lipo cream	V112180607EL	1
Noweda/Actavis	Abitima® clinic body cream	90118	2
Noweda/BDF	Eucerinum W/O basis	51630108WA	1
Noweda/Beiersdorf	Eucerinum W/O basis	83730308WA	1
Noweda/Beiersdorf	Eucerinum W/O basis	94930108	1
noweda/chiesi	Asche Basis® cream	52306A	1
Noweda/Chiesi	Asche Basis® cream	73386A	1
Noweda/Chiesi	Asche Basis® cream	82410A	1
Noweda/Chiesi	Asche Basis® cream	84424A	1
Noweda/Chiesi	Asche Basis® cream	94448A	1
Noweda/Galderma	Excipial® U Lipolotio	174756	1
Noweda/Galderma	Excipial® hydro cream	T091	2
Noweda/Galderma	Excipial® U Lipolotio	V121	1
Noweda/Jenapharm	Neribas® cream	YY00PF1	1
Noweda/Karo	Neribas® cream	YY052E2	1
Noweda/Leopharm	Neribas® cream	YY02H20	1
Noweda	Neuroderm® moisturising cream		2
Noweda	Excipial® hydro cream	1120114	1
Noweda	Asche Basis® cream	1449A	1
Noweda	Asche Basis® cream	1453A	2
Noweda	Asche Basis® cream	1455A	2
Noweda	Abitima® clinic face cream	146735	1
Noweda	Lipoderm® lotion	169310	1
Noweda	Excipial® hydro cream	1767001	2
Noweda	Excipial® hydro cream	1767002	1
Noweda	Excipial® lipo cream	1769017	1
Noweda	Abitima® clinic face cream	21101217	1

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Supplier	Substance	Batch	Spectra
Noweda	Asche Basis® cream	2459A	1
Noweda	Excipial® U Lipolotio	305489	1
Noweda	Excipial® U Lipolotio	311839	2
Noweda	Excipial® U Lipolotio	312417	3
Noweda	Excipial® U Lipolotio	312811	2
Noweda	Excipial® U Lipolotio	319844	1
Noweda	Excipial® U Lipolotio	327343	1
Noweda	Asche Basis® cream	3461A	2
Noweda	Excipial® lipo cream	50627	1
Noweda	Asche Basis® lotion	63980A	1
Noweda	Eucerinum W/O basis	72630108WA	4
Noweda	Excipial® hydro cream	767004	1
Noweda	Asche Basis® cream	81399A	1
Noweda	Asche Basis® cream	81404A	1
Noweda	Asche Basis® cream	82405A	1
Noweda	Asche Basis® cream	82410A	1
Noweda	Asche Basis® cream	83411A	2
Noweda	Asche Basis® cream	83412A	1
Noweda	Asche Basis® cream	83413A	1
Noweda	Eucerinum W/O basis	83730208WA	2
Noweda	Eucerinum W/O basis	83730308WA	1
Noweda	Eucerinum W/O basis	8373C208WA	1
Noweda	Asche Basis® cream	84417A	4
Noweda	Asche Basis® cream	84418A	3
Noweda	Asche Basis® cream	84424A	3
Noweda	Asche Basis® cream	91425A	1
Noweda	Asche Basis® cream	92434A	1
Noweda	Asche Basis® cream	92435A	2
Noweda	Asche Basis® cream	92436A	4
Noweda	Asche Basis® cream	92440A	1
Noweda	Asche Basis® cream	92441A	1
Noweda	Asche Basis® cream	92442A	2
Noweda	Asche Basis® lotion	93103A	4
Noweda	Asche Basis® cream	93447A	1
Noweda	Eucerinum W/O basis	94930108	2
Noweda	Eucerinum W/O basis	94930208	2
Noweda	Eucerinum W/O basis	94930308	1
Noweda	Excipial® hydro cream	9767001	1
Noweda	Excipial® lipo cream	9769004	1
Noweda	Excipial® lipo cream	9769030	2
Noweda	Excipial® U Lipolotio	LOT50876	1
Noweda	Lipoderm® lotion	LOT50932	1
Noweda	Excipial® U Lipolotio	R261	1
Noweda	Excipial® hydro cream	VO51	1
Noweda	Neribas® cream	YY04FEJ	1
P&M Cosmetics GmbH & Co...	Dermatest base ointment	200419	2
P&M Cosmetics GmbH & Co...	Dermatest base ointment	280821	1
p&M Cosmetics GmbH	Dermatest base ointment	270623	1
P&M Cosmetics/AEP	Dermatest base ointment	270623	1
P&M Cosmetics/Alliance ...	Dermatest base ointment	152241	1
P&M Cosmetics/Alliance	Dermatest base ointment	160820	1
P&M Cosmetics/Alliance	Dermatest base ointment	260820	2
P&M Cosmetics/Anzag	Dermatest base ointment	122631	1
P&M Cosmetics/Anzag	Dermatest base ointment	40622	1
P&M Cosmetics/Fiebig	Dermatest base ointment	280821	2
P&M Cosmetics/Fiebig	Dermatest base ointment	40622	1
p&m cosmetics/gehe	Dermatest base ointment	200419	1
P&M Cosmetics/Noweda	Dermatest base ointment	301124	1
P&M Cosmetics	Dermatest base ointment	210915	1
P&M Cosmetics	Dermatest base ointment	260820	2

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Supplier	Substance	Batch	Spectra
P&M Cosmetics	Dermatest base ointment	280821	1
P&M/Alliance	Dermatest base ointment	121217	1
P&M/Alliance	Dermatest base ointment	190317	1
P&M	Dermatest base ointment	241115	1
Persano/Gehe	Abitima® clinic face cream	57792	1
Ph.Eur.8.0	Eucerinum W/O basis	41830108WA	1
Phoenix / Bios Medical	Excipial® U Lipolotio	329498	1
Phoenix WE 13.04.17 -7,...	Asche Basis® cream	63353A	2
Phoenix WE: 08.11.17 10...	Asche Basis® cream	71372A	1
Phoenix WE: 09.10.17 50...	Asche Basis® cream	71368A	1
Phoenix/actavis	Abitima® clinic face cream	148460	1
Phoenix/Chiesi	Asche Basis® cream	33246A	1
Phoenix/Chiesi	Asche Basis® cream	61333A	1
Phoenix/Chiesi	Asche Basis® cream	64358A	1
Phoenix/Chiesi	Asche Basis® cream	73387A	1
Phoenix/Chiesi	Asche Basis® lotion	74091A	1
Phoenix/Chiesi	Asche Basis® cream	81399A	1
Phoenix/Chiesi	Asche Basis® lotion	91098A	1
Phoenix/Chiesi	Asche Basis® lotion	92101A	1
Phoenix/Galderma	Excipial® lipo cream	50567	1
Phoenix/Galderma	Excipial® hydro cream	T012	1
Phoenix/Nestle Skin Hea...	Excipial® U Lipolotio	324788	1
Phoenix/Spirig	Excipial® hydro cream	M015	1
Phoenix/Spirig	Excipial® U Lipolotio	N041	1
Phoenix/Spirig	Excipial® hydro cream	N044	1
Phoenix	Asche Basis® cream	11002A	1
Phoenix	Excipial® lipo cream	1769001	1
Phoenix	Asche Basis® cream	21018A	1
Phoenix	Asche Basis® cream	22019A	1
Phoenix	Dermatest base ointment	260820	1
Phoenix	Neribas® cream	3094	1
Phoenix	Excipial® U Lipolotio	319748	1
Phoenix	Neribas® cream	3229	1
Phoenix	Neribas® cream	3378	1
Phoenix	Asche Basis® lotion	52069A	1
Phoenix	Asche Basis® cream	53331A	1
Phoenix	Asche Basis® cream	54332A	1
phoenix	Eucerinum W/O basis	94930108	1
Phoenix	Eucerinum W/O basis	94930208	1
phoenix	Eucerinum W/O basis	94930308	1
Phoenix	Excipial® U Lipolotio	N105	1
Phoenix	Excipial® U Lipolotio	S091	1
Phoenix	Excipial® U Lipolotio	S138	2
Phoenix	Excipial® U Lipolotio	S148	1
Phoenix	Neribas® cream	YY02L84	3
Phoenix	Neribas® cream	YY08H20	1
Phönix / Jenapharm	Neribas® cream	YY01FX3	1
Phönix /Chiesi	Asche Basis® cream	81402A	1
Phönix Chiesi	Asche Basis® cream	93443A	3
Phönix Fontapharm	Fabitop® base cream	101601	1
phönix WE: 28.08.17 EK...	Asche Basis® cream	64365A	2
Phönix/ 09.03.2020	Asche Basis® cream	92441A	1
Phönix/ Chiesi	Asche Basis® cream	91425A	1
Phönix/ Nestle Skin Hea...	Excipial® U Lipolotio	314142	1
Phönix/Beiersdorf	Eucerinum W/O basis	94930108	7
Phönix/Beiersdorf	Eucerinum W/O basis	94930208	2
Phönix/Chiesi 07.12.20	Asche Basis® cream	24564A	1
Phönix/Chiesi	Asche Basis® lotion	91097A	3
Phönix/Chiesi	Asche Basis® lotion	92100A	2
Phönix/Fontapharm	Fabitop® base cream	GRWW2	1

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Supplier	Substance	Batch	Spectra
Phönix/Galderma	Excipial® U Lipolotio	332540	1
Phönix/Galderma	Excipial® hydro cream	9767005	1
Phönix/Galderma	Excipial® lipo cream	SO23	1
Phönix/Nestle Skin Health	Excipial® U Lipolotio	314603	1
Phönix/Sanofi	Dermatop® base cream	9F0874	1
Phönix/Sanofi	Dermatop® base cream	OF095A	1
Phönix/Spirig	Excipial® hydro cream	N034	1
PHÖNIX	Neuroderm® moisturising cream		1
Phönix	Asche Basis® cream	11002A	1
Phönix	Asche Basis® cream	14014A	1
Phönix	Hans Karrer Lipolotion Micro...	20007	1
phönix	Dermatest base ointment	270623	1
Phönix	Neribas® cream	3139	1
Phönix	Excipial® U Lipolotio	319844	1
Phönix	Asche Basis® cream	322344	1
Phönix	Excipial® U Lipolotio	324788	1
Phönix	Excipial® U Lipolotio	351894	1
PHÖNIX	Asche Basis® cream	62343A	1
PHÖNIX	Asche Basis® cream	73386A	1
Phönix	Excipial® hydro cream	767003	1
Phönix	Dermatop® base cream	7F072A	2
Phönix	Eucerinum W/O basis	80330108WA	1
Phönix	Asche Basis® cream	81404A	1
Phönix	Dermatop® base cream	8F076A	1
PHÖNIX	Asche Basis® lotion	91098A	1
Phönix	Eucerinum W/O basis	94930108	1
Phönix	Fabitop® base cream	GLWD3	1
PHÖNIX	Excipial® U Lipolotio	T063	1
Phönix	Excipial® hydro cream	V011	1
PHÖNIX	Excipial® U Lipolotio	V039	1
PHÖNIX	Excipial® U Lipolotio	V105	1
Phönix	Neribas® cream	YY0431J	1
Phönix	Neribas® cream	YY04EYL	1
Phönix	Neribas® cream	YY04FEJ	1
PhönixWE:3.02.2017 EK...	Asche Basis® cream	63350A	1
Pm Cosmetica/Gehe	Dermatest base ointment	280821	2
Puren / Gehe	Abitima® clinic face cream	174292	1
Puren / Phoenix	Abitima® clinic face cream	22100374	1
Puren / Phönix	Abitima® clinic face cream	169357	1
Puren / Phönix	Abitima® clinic face cream	171872	1
Puren / Phönix	Abitima® clinic face cream	174418	1
Puren / Phönix	Abitima® clinic face cream	20101760	1
Puren / Sanacorp	Abitima® clinic body cream	180125	2
Puren Ph./Gehe	Abitima® clinic body cream	131118	1
Puren Pharm/Phoenix	Abitima® clinic body cream	120119	1
Puren Pharm/Phoenix	Abitima® clinic body cream	130319	1
Puren Pharm/Phoenix	Abitima® clinic body cream	241118	2
Puren Pharm/Phönix	Abitima® clinic body cream	1311118	1
Puren Pharm/Phönix	Abitima® clinic body cream	251118	10
Puren Pharm/Phönix	Abitima® clinic body cream	261118	12
Puren Pharma / Kehr	Abitima® clinic body cream	18012G	1
Puren Pharma / Phönix	Abitima® clinic body cream	251118	2
Puren Pharma / Sanacorp	Abitima® clinic face cream	170180	5
Puren Pharma / Sanacorp	Abitima® clinic body cream	261118	1
Puren Pharma GmbH & Co....	Abitima® clinic face cream	174418	1
PUREN Pharma GmbH &CoKG...	Abitima® clinic body cream	90118	1
Puren Pharma GmbH / Kehr	Abitima® clinic body cream	131118	2
Puren Pharma GmbH / Lie...	Abitima® clinic body cream	90118	2
Puren Pharma GmbH/Phoenix	Abitima® clinic body cream	120319	1

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Supplier	Substance	Batch	Spectra
Puren Pharma GmbH	Abitima® clinic body cream	131118	2
Puren Pharma GmbH	Abitima® clinic body cream	13118	1
Puren Pharma GmbH	Abitima® clinic body cream	180125	1
Puren Pharma GmbH	Abitima® clinic body cream	180126	2
Puren Pharma GmbH	Abitima® clinic body cream	261118	1
Puren Pharma/ Gehe EK 4...	Abitima® clinic face cream	21101217	1
Puren Pharma/ Gehe EK 4...	Abitima® clinic face cream	174292	1
Puren Pharma/Anzag	Abitima® clinic body cream	180007	5
Puren Pharma/GEHE	Abitima® clinic body cream	120119	5
Puren Pharma/Noweda	Abitima® clinic body cream	90118	1
Puren Pharma/Phönix	Abitima® clinic body cream	185394	1
Puren Pharma/Sanacorp	Abitima® clinic body cream	180126	1
Puren Pharma/Spangro	Abitima® clinic face cream	174292	2
Puren Pharma	Abitima® clinic body cream	120319	1
Puren Pharma	Abitima® clinic face cream	169357	1
Puren Pharma	Abitima® clinic body cream	180126	1
Puren PharmaGmbH/Noweda	Abitima® clinic body cream	20118	2
Puren/ Alliance	Abitima® clinic body cream	261118	1
Puren/ Phoenix	Abitima® clinic body cream	180125	1
Puren/AHCA	Abitima® clinic face cream	164225	1
Puren/G	Abitima® clinic face cream	21101170	1
Puren/Gehe	Abitima® clinic body cream	185433	1
Puren/Gehe	Abitima® clinic face cream	20101613	1
Puren/Noweda	Abitima® clinic body cream	120319	2
Puren/Noweda	Abitima® clinic body cream	20118	1
Puren/Phoenix	Abitima® clinic body cream	130118	1
Puren/Phoenix	Abitima® clinic body cream	130319	1
Puren/Phoenix	Abitima® clinic body cream	261118	1
Puren	Abitima® clinic face cream	169356	1
Puren	Abitima® clinic body cream	251118	1
Roche/AHD	Abitima® clinic body cream	142620	1
Römerapo.	Excipial® hydro cream	R011	2
Rondell Apotheke	Eucerinum W/O basis	51630108WA	1
Sanacoro W.E:01.03.18 ...	Asche Basis® cream	72378A	1
Sanacoro W.E:01.03.18 ...	Asche Basis® cream	72379A	2
Sanacorp /100ml	Asche Basis® cream	72382A	2
Sanacorp EK:8,07 EUR...	Asche Basis® cream	64363A	1
Sanacorp EK:8,07 EUR...	Asche Basis® cream	64364A	1
sanacorp / Nestle	Excipial® U Lipolotio	174800	1
Sanacorp / Wolff	Asche Basis® cream	82A05A	1
Sanacorp /Chiesi	Asche Basis® cream	84418A	1
Sanacorp W.E: 02.02.18 ...	Asche Basis® cream	72377A	1
Sanacorp WE 20.02.17 -7...	Asche Basis® cream	63351A	3
Sanacorp WE 25.02.17 -1...	Excipial® U Lipolotio	LOTS122	2
SANACORP/ PUREN Pharma	Abitima® clinic face cream	174292	1
SANACORP/ Puren	Abitima® clinic body cream	120319	1
SANACORP/ Puren	Abitima® clinic body cream	20118	2
Sanacorp/Beiersdorf	Eucerinum W/O basis	80330108WA	3
Sanacorp/Beiersdorf	Eucerinum W/O basis	94930108	1
Sanacorp/Galderma	Excipial® U Lipolotio	312417	1
Sanacorp/Nestlé Skin Care	Excipial® U Lipolotio	318718	1
Sanacorp/Nestlé Skin Care	Excipial® U Lipolotio	320973	1
Sanacorp	Neuroderm® moisturising cream		2
Sanacorp	Abitima® clinic body cream	12015/110/12	1
Sanacorp	Abitima® clinic body cream	140113	1
Sanacorp	Abitima® clinic face cream	20101760	1
Sanacorp	Abitima® clinic body cream	210612	1
Sanacorp	Excipial® U Lipolotio	335695	1
Sanacorp	Abitima® clinic body cream	51112	1
Sanacorp	Asche Basis® cream	53327A	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Abitima® clinic body cream	70512	1
Sanacorp	Dermatest base ointment	70615	1
Sanacorp	Eucerinum W/O basis	72630108WA	1
Sanacorp	Excipial® lipo cream	769013	6
Sanacorp	Eucerinum W/O basis	80330108WA	1
Sanacorp	Asche Basis® lotion	82092A	2
Sanacorp	Asche Basis® cream	83412A	1
Sanacorp	Asche Basis® lotion	84096	1
SANACORP	Asche Basis® cream	84417A	2
Sanacorp	Asche Basis® cream	91426A	2
SANACORP	Asche Basis® cream	92435A	1
Sanacorp	Eucerinum W/O basis	94930208	1
Sanacorp	Excipial® hydro cream	LOTN011	1
Sanacorp	Excipial® lipo cream	LOTN016	1
Sanacorp	Excipial® hydro cream	LOTV071	1
Sanacorp	Excipial® lipo cream	M027	1
Sanacorp	Excipial® hydro cream	N011	1
Sanacorp	Neribas® cream	YY0431J	3
Sanofi / Gehe	Dermatop® base cream	4F046A	1
Sanofi / Phönix	Dermatop® base cream	8F082A	1
Sanofi / Phönix	Dermatop® base cream	94090A	1
Sanofi / Phönix	Dermatop® base cream	9F087A	1
Sanofi / Phönix	Dermatop® base cream	9F090A	3
Sanofi / Phönix	Dermatop® base cream	f092A	1
Sanofi / Phönix	Dermatop® base cream	F092A	2
Sanofi / Phönix	Dermatop® base cream	F096A	1
Sanofi / Phönix	Dermatop® base cream	F098B	1
Sanofi / Phönix	Dermatop® base cream	F92A	1
Sanofi / Phönix	Dermatop® base cream	OF094A	1
Sanofi / Phönix	Dermatop® base cream	OF096A	2
Sanofi /Noweda	Dermatop® base cream	F098A	1
Sanofi Aventis/Sanacorp	Dermatop® base cream	9F089A	1
Sanofi Aventis	Dermatop® base cream	4F046A	1
Sanofi/Alliance	Dermatop® base cream	F096A	1
Sanofi/AllianceHealthcare	Dermatop® base cream	F091A	2
Sanofi/Anzag	Dermatop® base cream	5F051A	1
Sanofi/Anzag	Dermatop® base cream	5F056A	1
Sanofi/Gehe	Dermatop® base cream	4F050A	1
Sanofi/Jenne	Dermatop® base cream	1F107A	1
Sanofi/Noweda	Dermatop® base cream	5F056A	1
Sanofi/Phönix	Dermatop® base cream	1F107A	1
Sanofi/Phönix	Dermatop® base cream	4F046A	1
Sanofi/Phönix	Dermatop® base cream	5F051A	1
Sanofi/Phönix	Dermatop® base cream	7F069A	1
Sanofi/Phönix	Dermatop® base cream	7F071A	1
Sanofi/Phönix	Dermatop® base cream	7F073A	2
Sanofi/Phönix	Dermatop® base cream	8F074A	2
Sanofi/Phönix	Dermatop® base cream	8F075A	1
Sanofi/Phönix	Dermatop® base cream	8F076A	1
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	8F082A	1
Sanofi/Phönix	Dermatop® base cream	8F082B	1
Sanofi/Phönix	Dermatop® base cream	8F083A	3
Sanofi/Phönix	Dermatop® base cream	8F084A	3
Sanofi/Phönix	Dermatop® base cream	9F086A	1
Sanofi/Phönix	Dermatop® base cream	9F087A	1
Sanofi/Phönix	Dermatop® base cream	9F089A	1

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Supplier	Substance	Batch	Spectra
Sanofi/Sanacorp	Dermatop® base cream	7F071A	1
Sanofi	Dermatop® base cream	4F046A	1
Sanofi	Dermatop® base cream	8F084A	4
Sanofi	Dermatop® base cream	F092A	1
Sanofi	Dermatop® base cream	F096A	1
Sanofi	Dermatop® base cream	OF092A	1
Sanofi-Aventis/Gehe	Dermatop® base cream	5F051A	1
Sanofi-Aventis/Phönix	Dermatop® base cream	6F065A	1
Sino Phyto	Asche Basis® cream	74394A	1
Sino Phyto	Asche Basis® cream	92436A	2
Spangropharm	Fabitop® base cream	1016022	1
Spangropharm	Fabitop® base cream	101603	1
Spangropharm	Fabitop® base cream	52002	1
Spangropharm	Asche Basis® cream	82093A	1
Spangropharm	Fabitop® base cream	GLWD5	3
Spangropharm	Neribas® cream	YY043TY	1
Spierig Pharma AG/ Anzag	Excipial® hydro cream	LOTNO34	1
Spierig Pharma AG/ Anzag	Excipial® hydro cream	LOTR013	1
Spierig Pharma AG/ Sana...	Excipial® lipo cream	LOTNO21	2
Spierig/Gehe	Excipial® hydro cream	R014	1
Spirg	Excipial® U Lipolotio	NO86	1
Spirig (Galderma)	Excipial® hydro cream	T011	1
Spirig (Galderma)	Excipial® hydro cream	T012	2
Spirig (Galderma)	Excipial® lipo cream	T061	1
Spirig (Galderma)	Excipial® hydro cream	V011	2
Spirig / Anzag	Excipial® hydro cream	813993/09	1
Spirig / Anzag	Excipial® hydro cream	813993/10	1
Spirig / Anzag	Excipial® lipo cream	813994/09	1
Spirig / Anzag	Excipial® hydro cream	LOTNO43	1
Spirig / Anzag	Excipial® lipo cream	M017	1
Spirig / Anzag	Excipial® lipo cream	M042	3
Spirig / Anzag	Excipial® U Lipolotio	M182	1
Spirig / Anzag	Excipial® lipo cream	N018	3
Spirig / Anzag	Excipial® U Lipolotio	N032	1
Spirig / Anzag	Excipial® hydro cream	N034	1
Spirig / Anzag	Excipial® U Lipolotio	N041	1
Spirig / Anzag	Excipial® lipo cream	NO18	1
Spirig / Galderma / Anzag	Excipial® U Lipolotio	169010	1
Spirig / Galderma / Anzag	Excipial® U Lipolotio	170615	1
Spirig / Gehe	Excipial® hydro cream	N011	1
Spirig / Noweda	Excipial® hydro cream	N035	1
Spirig / Sanacorp	Excipial® U Lipolotio	R041	1
Spirig /Gehe	Excipial® lipo cream	LOTNO21	2
Spirig /Gehe	Excipial® hydro cream	LOTNO44	1
Spirig /Gehe	Excipial® lipo cream	LOTRO12	1
Spirig /Gehe	Excipial® lipo cream	R012	1
Spirig Pharma / Noweda	Excipial® U Lipolotio	S141	1
Spirig Pharma AG/Allian...	Excipial® lipo cream	N018	1
Spirig Pharma AG/Allian...	Lipoderm® lotion	N041	1
Spirig Pharma AG/Allian...	Lipoderm® lotion	NO41	1
Spirig Pharma AG/Allian...	Lipoderm® lotion	R011	4
Spirig Pharma AG/Allian...	Lipoderm® lotion	R023	8
Spirig Pharma AG/Allian...	Lipoderm® lotion	R044	3
Spirig Pharma AG/GEHE	Excipial® hydro cream	R011	1
Spirig Pharma AG/GEHE	Excipial® lipo cream	R012	1
Spirig Pharma AG	Excipial® hydro cream	813993/12	1
Spirig Pharma AG	Excipial® lipo cream	M042	1
Spirig Pharma AG	Lipoderm® lotion	N041	1
Spirig Pharma AG	Excipial® hydro cream	R025	5
Spirig Pharma AG	Excipial® U10 Lipolotio	V082	1

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Supplier	Substance	Batch	Spectra
Spirig Pharma Europe GmbH	Excipial® lipo cream	R026	1
Spirig Pharma/ G	Excipial® hydro cream	S053	1
Spirig Pharma/ Noweda	Excipial® hydro cream	N042	2
Spirig Pharma/Galderma	Excipial® U Lipolotio	327343	1
Spirig Pharma/Galderma	Excipial® U Lipolotio	332540	2
Spirig Pharma/Gehe	Excipial® hydro cream		1
Spirig Pharma/Kehr	Excipial® U Lipolotio	T156	2
Spirig Pharma	Excipial® U Lipolotio	170615	2
Spirig Pharma	Excipial® U Lipolotio	174756	2
Spirig Pharma	Excipial® U Lipolotio	305489	3
Spirig Pharma	Excipial® hydro cream	50782	2
Spirig Pharma	Excipial® hydro cream	813993/10	1
Spirig Pharma	Excipial® lipo cream	813994/09	2
Spirig Pharma	Excipial® hydro cream	LON014	1
Spirig Pharma	Excipial® U Lipolotio	LOTK131	1
Spirig Pharma	Excipial® U Lipolotio	LOTN013	1
Spirig Pharma	Excipial® U Lipolotio	M134	1
Spirig Pharma	Excipial® hydro cream	N011	1
Spirig Pharma	Excipial® hydro cream	N013	1
Spirig Pharma	Excipial® hydro cream	N044	1
Spirig Pharma	Excipial® U Lipolotio	S122	1
Spirig Pharma	Excipial® lipo cream	T021	1
Spirig Pharma	Lipoderm® lotion	V012	1
Spirig Pharma	Excipial® U Lipolotio	V053	1
Spirig Pharma	Excipial® U Lipolotio	V082	1
Spirig Pharma	Excipial® U Lipolotio	V141	2
Spirig/ Noweda	Excipial® U Lipolotio	S225	1
Spirig/AHD	Lipoderm® lotion	LOTN041	1
Spirig/AHD	Excipial® U Lipolotio	lotno86	1
Spirig/AHD	Excipial® lipo cream	M017	1
Spirig/AHD	Excipial® U10 Lipolotio	M025	1
Spirig/AHD	Excipial® lipo cream	M041	2
Spirig/AHD	Lipoderm® lotion	M065	4
Spirig/AHD	Excipial® U Lipolotio	M085	1
Spirig/AHD	Excipial® lipo cream	N018	2
Spirig/AHD	Lipoderm® lotion	N041	1
Spirig/AHD	Excipial® U Lipolotio	N058	1
Spirig/AllianceHC	Lipoderm® lotion	S021	3
Spirig/Anzag	Excipial® hydro cream	LOTM041	1
Spirig/Anzag	Excipial® hydro cream	N035	1
Spirig/Anzag	Excipial® lipo cream	R011	1
Spirig/Anzag	Excipial® lipo cream	S023	1
Spirig/Anzag	Excipial® lipo cream	S031	1
Spirig/Fiebig	Excipial® hydro cream	N013	1
Spirig/Fiebig	Excipial® U Lipolotio	S143	1
Spirig/Galderma	Excipial® U Lipolotio	R146	1
Spirig/Galderma	Excipial® U Lipolotio	R156	2
Spirig/Gehe	Excipial® hydro cream		3
Spirig/Gehe	Excipial® hydro cream	LOTR031	2
Spirig/Gehe	Excipial® hydro cream	M012	1
Spirig/Gehe	Excipial® U Lipolotio	M102	2
Spirig/Gehe	Excipial® U Lipolotio	M146	1
Spirig/Gehe	Excipial® U Lipolotio	M182	1
Spirig/Gehe	Excipial® lipo cream	R012	1
Spirig/Gehe	Excipial® lipo cream	R026	1
Spirig/Gehe	Excipial® U Lipolotio	R114	1
Spirig/Gehe	Excipial® U Lipolotio	R262	1
Spirig/Gehe	Lipoderm® lotion	S041	1
Spirig/Kehr	Excipial® U Lipolotio	V038	1
Spirig/Noweda	Excipial® hydro cream	50782	1

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Supplier	Substance	Batch	Spectra
Spirig/Noweda	Excipial® hydro cream	N043	3
Spirig/Noweda	Excipial® U Lipolotio	N061	1
Spirig/Otto	Excipial® lipo cream	50627	1
Spirig/Phoenix	Excipial® lipo cream	M042	2
Spirig/Phönix	Excipial® lipo cream	4622	1
Spirig/Phönix	Excipial® lipo cream	R012	2
Spirig/Phönix	Excipial® hydro cream	R013	1
Spirig/Phönix	Excipial® hydro cream	R014	1
Spirig/Phönix	Excipial® U Lipolotio	R033	1
Spirig/Phönix	Excipial® lipo cream	R042	1
Spirig/Würmtal-Apotheke	Excipial® U Lipolotio	R145	2
spirig	Excipial® lipo cream		1
Spirig	Excipial® U Lipolotio	169838	1
spirig	Lipoderm® lotion	4622	1
Spirig	Excipial® U Lipolotio	50450	1
spirig	Excipial® hydro cream	813993/10	1
spirig	Excipial® lipo cream	813994/09	1
Spirig	Excipial® hydro cream	K013	1
Spirig	Excipial® lipo cream	K021	1
Spirig	Lipoderm® lotion	LOTR011	1
Spirig	Excipial® U Lipolotio	LOTT057	1
spirig	Excipial® lipo cream	M016	1
spirig	Excipial® hydro cream	M034	1
spirig	Excipial® hydro cream	M041	2
spirig	Excipial® lipo cream	M042	2
Spirig	Excipial® U Lipolotio	M091	1
spirig	Excipial® U Lipolotio	M142	1
spirig	Excipial® lipo cream	N018	4
spirig	Excipial® lipo cream	N021	5
Spirig	Excipial® lipo cream	N021	1
spirig	Excipial® hydro cream	N034	2
spirig	Excipial® hydro cream	N043	2
Spirig	Excipial® hydro cream	N043	1
spirig	Excipial® hydro cream	N045	2
spirig	Excipial® U Lipolotio	N058	3
spirig	Excipial® lipo cream	N061	3
Spirig	Excipial® U Lipolotio	N123	1
spirig	Excipial® U Lipolotio	NO13	1
spirig	Excipial® hydro cream	No14	1
Spirig	Excipial® hydro cream	NO35	1
spirig	Excipial® U Lipolotio	NO86	1
Spirig	Lipoderm® lotion	R011	2
spirig	Excipial® lipo cream	R012	3
Spirig	Excipial® lipo cream	R012	4
spirig	Excipial® hydro cream	R013	2
Spirig	Excipial® hydro cream	R013	1
spirig	Excipial® hydro cream	R014	2
Spirig	Lipoderm® lotion	R023	2
spirig	Excipial® U Lipolotio	R037	1
spirig	Excipial® lipo cream	r042	1
Spirig	Excipial® U Lipolotio	R047	1
spirig	Excipial® hydro cream	s025	1
Spirig	Excipial® hydro cream	S025	6
Spirig	Lipoderm® lotion	S041	2
Spirig	Excipial® U Lipolotio	T149	1
SpirigPharm/Noweda	Lipoderm® lotion	LOT50932	1
SpirigPharma	Lipoderm® lotion	S041	1
Sprig (Galderma)/ G	Excipial® U Lipolotio	S123	1
Spring Pharma AG/Sanacorp	Excipial® U Lipolotio	318628	2
Spririg / Noweda	Excipial® hydro cream	S041	5

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Supplier	Substance	Batch	Spectra
St. Martin/Taoasis	Base cream Taoasis	180924-8114	1
Taoasis / Sanacorp	Base cream Taoasis	SAP2792-2216	1
Taoasis GmbH/ Taoasis	Base cream Taoasis	190916-9182	1
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	200303-9344	1
Taoasis GmbH	Base cream Taoasis	200708-0079	1
Taoasis GmbH	Base cream Taoasis	201028-0197	1
Taoasis/ Noweda	Base cream Taoasis	200708-0079	1
Taoasis/ Noweda	Base cream Taoasis	SAP2638-2019	1
Taoasis/Noweda	Base cream Taoasis	SAP3344-3115	1
Taoasis/Phoenix	Base cream Taoasis	180718-7100	1
Taoasis/Phoenix	Base cream Taoasis	210716-1124	1
Taoasis/Sanacorp	Base cream Taoasis	170317-7031	3
Taoasis/Sanacorp	Base cream Taoasis	170517-7100	2
Taoasis/Sanacorp	Base cream Taoasis	171127-7290	10
Taoasis/Sanacorp	Base cream Taoasis	180515-8030	1
Taoasis/Sanacorp	Base cream Taoasis	1807187100	1
Taoasis/Sanacorp	Base cream Taoasis	180924-8114	1
Taoasis/Taoasis	Base cream Taoasis	210309-0343	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	1
Taoasis	Base cream Taoasis	170317-7031	1
Taoasis	Base cream Taoasis	170517-7100	1
Taoasis	Base cream Taoasis	171127-7290	1
taoasis	Base cream Taoasis	180307-8030	1
Taoasis	Base cream Taoasis	181204-8333	1
Taoasis	Base cream Taoasis	190920-9182A	1
Taoasis	Base cream Taoasis	200303-9344	1
Taoasis	Base cream Taoasis	200708-0079	1
Taoasis	Base cream Taoasis	210716-1124	1
THC/ Phönix Pharma Eink...	Asche Basis® cream	129880	1
THC/Noweda	Fabitop® base cream	1016022	1
WE Sanacorp	Asche Basis® cream	61341A	1
WE: Phoenix 07.10.2016 ...	Asche Basis® cream	61340A	1
WE: Phoenix 23.09.2016 ...	Asche Basis® cream	61339A	1
WE:Phönix28.07.2016 E...	Asche Basis® cream	61336A	1
Wolff/ Sanacorp	Asche Basis® cream	810201	1
Wolff/Gehe	Asche Basis® cream	64365A-20171106Ma10	1
Wolff/Gehe	Asche Basis® cream	71366A	1
Wolff	Excipial® lipo cream	S031	1

- 11 290 spectra from 1129 *Apo-Ident* customers from a total of 3782 batches from a further 137 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 *Hydrophilic market-ready products* 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 *Hydrophilic*

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market-ready products 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	4530	0	24 025
Type B	0	2972	98	22 035
Type C	0	3984	159	11 255

The substance/substance group *Hydrophilic market-ready products* 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 % (> 99.9635 %)	100.0000 % (> 99.8675 %)
Type B	100.0000 % (> 99.9493 %)	96.8078 % (> 96.7101 %)
Type C	100.0000 % (> 99.0135 %)	96.1622 % (> 96.0898 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Hydrophilic market-ready products* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
ALLERGIKA®-Lipolotio urea 5% F	12.19	–
Dimeticone ointment 10% SR	12.63	–
ALLERGIKA® – Eyelid cream MED	14.36	–
Dexeryl®	15.67	–
Neuroderm® moisturising cream lipo	17.01	–
La Roche-Posay Toleriane	19.83	–
ALLERGIKA® – Nachtkerzenöl Creme 20%	26.50	–
Amciderm® Base cream	28.10	–
Dermatop® base ointment	31.96	–
Dermifant® kids cream	36.80	–
Nourivan™ Antiox	38.85	–

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

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
30634	30634	0.00	39.00
30635	30635	0.00	33.80
30713	30713	0.00	33.90
30722	30722	0.00	31.00
30725	30725	0.00	39.42
30726	30726	0.00	34.77
30732	30732	0.00	41.79
30733	30733	0.00	34.40
30775	30775	0.00	36.32
30828	30828	0.00	21.52
30845	30845	0.00	14.28
30993	30993	0.00	44.00
31041	31041	0.00	20.24
31050	31050	0.00	38.75
31058	31058	0.00	41.24
31061	31061	0.00	42.43
31066	31066	0.00	31.17
31067	31067	0.00	36.46
31068	31068	0.00	26.90
31070	31070	0.00	19.21
31072	31072	0.00	40.81
31082	31082	0.00	60.73
31085	31085	0.00	38.71
31088	31088	0.00	45.60
31089	31089	0.00	44.70
31095	31095	0.00	36.93
31102	31102	0.00	26.80
31115	31115	0.00	22.80
31234	31234	0.00	34.40
31236	31236	0.00	37.88
31280	31280	0.00	41.63
31281	31281	0.00	30.71
31307	31307	0.00	28.12
31308	31308	0.00	45.99
31309	31309	0.00	49.25
31511	31511	0.00	30.15
31520	31520	0.00	47.86
31535	31535	0.00	36.64
31539	31539	0.00	21.14
31576	31576	0.00	58.12
31578	31578	0.00	30.22
31627	31627	0.00	19.17
31730	31730	0.00	26.99
31761	31761	0.00	26.77
31772	31772	0.00	19.90
31869	31869	0.00	32.66
31870	31870	0.00	45.84
31873	31873	0.00	25.51
31874	31874	0.00	37.31

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31950	31950	0.00	19.85
32177	32177	0.00	32.97
32178	32178	0.00	41.67
32767	32767	0.00	30.81
32916	32916	0.00	39.94
32997	32997	0.00	40.13
33039	33039	0.00	19.71
33194	33194	0.00	25.30
33195	33195	0.00	26.16
33207	33207	0.00	46.79
33208	33208	0.00	31.38
33213	33213	0.00	26.02
33221	33221	0.00	41.01
33270	33270	0.00	41.51
33636	33636	0.00	43.51
33737	33737	0.00	24.13
33793	33793	0.00	15.57
33968	33968	0.00	41.59
33969	33969	0.00	40.98
34043	34043	0.00	46.04
34044	34044	0.00	21.75
34117	34117	0.00	34.24
34119	34119	0.00	22.90
34359	34359	0.00	41.37
34360	34360	0.00	14.79
35149	35149	0.00	13.82
35502	35502	0.00	26.10
35504	35504	0.00	27.99
35573	35573	0.00	22.42
35583	35583	0.00	36.18
35585	35585	0.00	40.96
35586	35586	0.00	43.27
35813	31576	8.30	52.04
36037	36037	0.00	29.69
36389	36389	0.00	18.58
36608	36608	0.00	30.58
36610	36610	0.00	34.10
36613	36613	0.00	35.51
36616	36616	0.00	38.84
36619	36619	0.00	37.62
36620	36620	0.00	40.05
36724	36724	0.00	22.60
36728	36728	0.00	24.69
36729	36729	0.00	24.41
36759	36759	0.00	25.95
36760	36760	0.00	34.64
36761	36761	0.00	34.16
36770	36770	0.00	27.84
36774	36774	0.00	18.40
37415	37415	0.00	32.47
37419	37419	0.00	18.01

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
37451	37451	0.00	21.40
37452	37452	0.00	37.71

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Immortelle oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30450-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	4	2	5

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Immortelle oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 28 375 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 5 batches from the substance/substance group *Immortelle oil*.
- 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
Taoasis	Immortelle oil	7750IT-L08	1
Taoasis	Immortelle oil	L03111DN	1
Taoasis	Immortelle oil	L14717DNJ-132	1
Taoasis	Immortelle oil	L14717DNJ-3017	1
Taoasis	Immortelle oil	L38914DN-118878	2

- 15 427 spectra from 1165 *Apo-Ident* customers from a total of 5019 batches from a further 158 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	180	0	28 375
Type B	0	80	0	26 021
Type C	0	6	0	15 427

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 % (> 99.9638 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9734 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Immortelle oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Melissa oil	14.65	–
Ginger oil	15.75	–
Vetiver bourbon oil	20.76	–
Citus oil	30.40	–
Cypress oil	31.02	–
Myrtle oil	31.66	–
Lemon grass oil	33.12	–
Cedar wood oil	33.53	–
Chamomile (essential oil)	34.84	–
Marjoram oil	37.20	–
Spearmint oil	38.58	–
Swiss pine oil	41.35	–
Dwarf pine oil	43.24	–
Patchouli oil	45.38	–
Carrot seed oil	48.66	–
Manuka oil	49.15	–
Hyssop oil	49.25	–

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.

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	25.06
32069	32069	0.00	20.86
33727	33727	0.00	28.86
34383	34383	0.00	26.69

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

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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 2.5-2023-04

Validated substance/substance group	**Juniper oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31559-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Juniper oil

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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 oil	4	3	2

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Juniper oil	4155-116757	31559	60	not required
Taoasis	Juniper oil	4155-120900	31687	60	not required
Taoasis	Juniper oil	02JB0B-126047	32809	40	not required
Taoasis	Juniper oil	9321-14903	37674	40	not required

Validation samples

A total of 70 089 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 *Juniper oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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 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 oil	00497L26	34398	40
Taoasis	Juniper oil	02JB0B-127283	32932	40
Taoasis	Juniper oil	1713-128196	33651	40

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- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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 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 oil	16160706	1
Taoasis	Juniper oil	155-118896	1

- 15 431 spectra from 1165 *Apo-Ident* customers from a total of 5022 batches from a further 158 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 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 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	28 355
Type B	0	111	9	25 981
Type C	0	2	0	15 431

The substance/substance group *Juniper 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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9510 %)	92.5000 % (> 90.0000 %)
Type C	100.0000 % (> 98.9905 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Juniper oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Frankincense oil	17.82	–
Dwarf pine oil	17.82	–
Spearmint oil	23.36	–
Pine silvestris oil	23.93	–
Spruce needle oil	29.20	–
Angelica root oil	29.67	–
Silver fir oil	29.94	–
Swiss pine oil	34.98	–
Yarrow oil	38.68	–
Cypress oil	38.88	–
Matricaria oil, morrocan	44.87	–
Marjoram oil	45.05	–
Citus oil	45.34	–

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

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	24.59
31687	31687	0.00	26.20
32809	32809	0.00	22.31
37674	37674	0.00	17.71

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**La Roche-Posay Cold Cream Naturel**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30829-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

La Roche-Posay Cold Cream Naturel

Special notes

When selecting the *La Roche-Posay Cold Cream Naturel* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
La Roche-Posay Cold Cream Naturel	3	2	4

Second-stage model

For differentiation of the substance/substance group *La Roche-Posay Cold Cream Naturel* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *La Roche-Posay Cold Cream Naturel*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
La Roche-Posay	La Roche-Posay Cold Cream Na…	54J01P	30829	40	not required
La Roche-Posay	La Roche-Posay Cold Cream Na…	54K31P	31074	40	not required
La Roche-Posay	La Roche-Posay Cold Cream Na…	54LN1P	31765	60	not required

Validation samples

A total of 70 089 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 *La Roche-Posay Cold Cream Naturel*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *La Roche-Posay Cold Cream Naturel*.
- 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
La Roche-Posay	La Roche-Posay Cold Cream Na…	54M51P	33262	40
La Roche-Posay	La Roche-Posay Cold Cream Na…	54P61P	33984	40

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 3 *Apo-Ident* customers from 4 batches from the substance/substance group *La Roche-Posay Cold Cream Naturel*.
- 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
Gehe	La Roche-Posay Cold Cream Na…	54M91P	1
La Roche-Posay	La Roche-Posay Cold Cream Na…	54M01P	1
La Roche-Posay	La Roche-Posay Cold Cream Na…	54M11P	1
La Roche-Posay	La Roche-Posay Cold Cream Na…	54M91P	1
Mea-SanacorpWE10.02.201…	La Roche-Posay Cold Cream Na…	LOT54M91P	1

- 15 428 spectra from 1165 *Apo-Ident* customers from a total of 5020 batches from a further 158 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 *La Roche-Posay Cold Cream Naturel* 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 *La Roche-Posay Cold Cream Naturel* 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	28 415
Type B	0	80	0	26 021
Type C	0	5	0	15 428

The substance/substance group *La Roche-Posay Cold Cream Naturel* 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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9751 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *La Roche-Posay Cold Cream Naturel* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Stomahesive® adhesive paste	50.85	–

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

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
30829	30829	0.00	80.19
31074	31074	0.00	83.87
31765	31765	0.00	83.54

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**La Roche-Posay Toleriane**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30827-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

La Roche-Posay Toleriane

Special notes

When selecting the *La Roche-Posay Toleriane* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
La Roche-Posay Toleriane	3	2	4

Second-stage model

For differentiation of the substance/substance group *La Roche-Posay Toleriane* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *La Roche-Posay Toleriane*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
La Roche-Posay	La Roche-Posay Toleriane	54J901	30827	40	not required
La Roche-Posay	La Roche-Posay Toleriane	54K500	31094	40	not required
La Roche-Posay	La Roche-Posay Toleriane	54N201	32563	40	not required

Validation samples

A total of 70 089 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 *La Roche-Posay Toleriane*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 435 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *La Roche-Posay Toleriane*.
- 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
La Roche-Posay	La Roche-Posay Toleriane	54N600	32759	40
La Roche-Posay	La Roche-Posay Toleriane	54P401	33983	40

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 2 *Apo-Ident* customers from 4 batches from the substance/substance group *La Roche-Posay Toleriane*.

- 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
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

- 15 426 spectra from 1165 *Apo-Ident* customers from a total of 5020 batches from a further 158 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 *La Roche-Posay Toleriane* 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 *La Roche-Posay Toleriane* 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	28 435
Type B	0	80	0	26 021
Type C	0	6	1	15 426

The substance/substance group *La Roche-Posay Toleriane* 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 % (> 99.9639 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9722 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *La Roche-Posay Toleriane* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Eucerinum W/O basis	18.88	–
DMS® base cream high classic	19.91	–
Neuroderm® moisturising cream	20.76	–
Abitima® clinic body cream	23.76	–
Excipial® U10 Lipolotio	23.82	–
Hans Karrer Lipocream MicroSilver	24.42	–
DMS® base cream classic	27.20	–
Base cream Taoasis	27.62	–
Asche Basis® lotion	30.12	–
Excipial® U Lipolotio	30.86	–
Asche Basis® cream	32.94	–
Lipoderm® lotion	35.08	–
Dimeticone ointment 10% SR	35.74	–
Base cream DVL-P	37.35	–
Neribas® cream	41.77	–
Linola® body milk	43.45	–
Hans Karrer Lipolotion MicroSilver	43.70	–
DMS® base cream high classic plus	45.74	–
Neuroderm® care lotion	47.42	–
ALLERGIKA® – Face cream MED	48.27	–
ALLERGIKA® – Eyelid cream MED	48.32	–
Excipial® hydro cream	52.40	–

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

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
30827	30827	0.00	30.71
31094	31094	0.00	25.24
32563	32563	0.00	30.15

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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 2.5-2023-04

Validated substance/substance group	**Lemon grass oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30661-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lemon grass oil; Cymbopoginis aetheroleum

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	5	4	23

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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
Taoasis	Lemon grass oil	130930-116754	31549	60	not required

Validation samples

A total of 70 089 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 *Lemon grass oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 28 335 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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.

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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

- 25 941 spectra from a total of 584 batches from further 209 substances. These spectra were recorded by *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.

- 26 spectra from 14 *Apo-Ident* customers from 24 batches from the substance/substance group *Lemon grass oil*.

- 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
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
Primavera/Sanacorp	Lemon grass oil	484A25	1
Primavera	Lemon grass oil	11401144	1
Primavera	Lemon grass oil	52A28	1
Primavera	Lemon grass oil	61E28	1
Taoasis	Lemon grass oil	104373-11249	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

- 15 407 spectra from 1165 *Apo-Ident* customers from a total of 5000 batches from a further 158 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	220	0	28 335
Type B	0	158	2	25 941
Type C	0	20	6	15 407

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 % (> 99.9637 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9509 %)	98.7500 % (> 96.8750 %)
Type C	100.0000 % (> 98.9668 %)	76.9231 % (> 65.3846 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Lemon grass oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	26.98	–
Cypress oil	29.37	–
Melissa oil	30.52	–
Carrot seed oil	31.01	–
Immortelle oil	31.84	–
Patchouli oil	32.87	–
Tea tree oil	38.93	–
Ginger oil	40.65	–
Myrtle oil	40.79	–
Vetiver bourbon oil	46.08	–
Cedar wood oil	50.17	–

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.

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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	30.52
31185	31185	0.00	35.49
31187	31187	0.00	32.87
31549	31549	0.00	32.17
36040	36040	0.00	32.52

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 2.5-2023-04

Validated substance/substance group	**Liniment ointments**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30731-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Liniment ointments; Amciderm® Base cream; Excipial® U Hydrolotio; Nourivan™ Antiox

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Liniment ointments	12	4	46

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Liniment ointments*:

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 Labo…	Excipial® U Hydrolotio	331554	35469	40	not required
Galderma Labo…	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
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

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 610 spectra of 13 reference samples from the substance/substance group *Liniment ointments*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.

- 27 945 spectra from a total of 593 batches from further 157 substances. These spectra were recorded by *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 by *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.

- 265 spectra of 8 reference samples from the substance/substance group *Liniment ointments*.

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- 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
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
Fagron	Nourivan™ Antiox	1503258	31958†	15
Fagron	Nourivan™ Antiox	1503258	32778	40
Fagron	Nourivan™ Antiox	1503258	32822	40
Fagron	Nourivan™ Antiox	1703842	33789†	10

- 25 836 spectra from a total of 582 batches from further 207 substances. These spectra were recorded by *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.

- 100 spectra from 42 *Apo-Ident* customers from 52 batches from the substance/substance group *Liniment ointments*.

- Among them are spectra of independent samples from 46 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Excipial® U Hydrolotio	378787	1
Allmiral/Gehe	Amciderm® Base cream	418321	1
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
Caelo	Excipial® U Hydrolotio	LOTR092	1
Fagron	Nourivan™ Antiox	150325	1
Fagron	Nourivan™ Antiox	1503258	3
Fagron	Amciderm® Base cream	23102017	1
Galderma / Alliance Hea...	Excipial® U Hydrolotio	340781	2
Galderma International ...	Excipial® U Hydrolotio	346815	1
Galderma International/...	Excipial® U Hydrolotio	V042	1
Galderma Laboratorium G...	Excipial® U Hydrolotio	340781	1
Galderma Laboratorium G...	Excipial® U Hydrolotio	344143	2
Galderma Laboratorium G...	Excipial® U Hydrolotio	344145	1
Galderma Laboratorium G...	Excipial® U Hydrolotio	357789	1
Galderma Laboratorium G...	Excipial® U Hydrolotio	365111	1
Galderma Laboratorium G...	Excipial® U Hydrolotio	318208	1
Galderma/ Fiebig	Excipial® U Hydrolotio	LOTV022	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
Galderma/ Gehe	Excipial® U Hydrolotio	LOTR053	1
Galderma/ Phoenix/ 07.1...	Excipial® U Hydrolotio	302972	1
Galderma/ Phoenix/ 09.0...	Excipial® U Hydrolotio	327533	1
Galderma/ Phoenix	Excipial® U Hydrolotio	324614	1
Galderma/ Phoenix	Excipial® U Hydrolotio	331554	4
Galderma/ Phoenix	Excipial® U Hydrolotio	344143	2
Galderma/ Phoenix	Excipial® U Hydrolotio	344145	1
Galderma/ Phönix	Excipial® U Hydrolotio	340781	1
Galderma/Alliance	Excipial® U Hydrolotio	365111	4
Galderma/Alliance	Excipial® U Hydrolotio	50723	1
Galderma/Alliance	Excipial® U Hydrolotio	T072	2
Galderma/Gehe	Excipial® U Hydrolotio	50723	1
Galderma/Gehe	Excipial® U Hydrolotio	S014	1
Galderma/Noweda	Excipial® U Hydrolotio	164957	1
Galderma/Noweda	Excipial® U Hydrolotio	324226	2
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
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	50857	1
Galderma	Excipial® U Hydrolotio	LOTR054	1
Galderma	Excipial® U Hydrolotio	T011	1
Galderma	Excipial® U Hydrolotio	V042	1
Galderna/Sanacorp	Excipial® U Hydrolotio	340781	1
Nestlé Skin Health / Sa...	Excipial® U Hydrolotio	324614	1
Nestle Skin Health/ Now...	Excipial® U Hydrolotio	324614	1
Nestle Skin Health/ San...	Excipial® U Hydrolotio	331554	1
Nestlé Skin Health/Gehe	Excipial® U Hydrolotio	324614	1
Nestlé Skin Health	Excipial® U Hydrolotio	315815	1
Nestlé Skin Health	Excipial® U Hydrolotio	331554	1
Nestle/ Phönix	Excipial® U Hydrolotio	331554	2
Netslé Skin Health/Gehe	Excipial® U Hydrolotio	324614	1
Noweda	Excipial® U Hydrolotio	S061	1
Phoenix/Spirig	Excipial® U Hydrolotio	M016	1
Phönix, Galderma, 09.04...	Excipial® U Hydrolotio	317160	1
Phönix	Excipial® U Hydrolotio	331554	1
PHÖNIX	Excipial® U Hydrolotio	50593	1
PHÖNIX	Excipial® U Hydrolotio	V051	1
SANACORP	Excipial® U Hydrolotio	172141	1
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/Gehe	Excipial® U Hydrolotio	R054	3
Spirig	Excipial® U Hydrolotio	N013	1
Spirig	Excipial® U Hydrolotio	N013	1

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- 15 333 spectra from 1165 *Apo-Ident* customers from a total of 4981 batches from a further 156 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 *Liniment 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 *Liniment 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	610	0	27 945
Type B	0	237	28	25 779
Type C	0	98	2	15 148

The substance/substance group *Liniment 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 % (> 99.9635 %)	100.0000 % (> 99.0164 %)
Type B	100.0000 % (> 99.9504 %)	89.4340 % (> 88.3019 %)
Type C	100.0000 % (> 98.9559 %)	98.0000 % (> 95.0000 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Liniment ointments* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Sebexol® basic pH 5 formula basis	8.80	–
Hans Karrer Hydrocream MicroSilver	10.51	–
Sebexol® cream lotion pH 5	11.06	–
Dimeticone ointment 10% SR	17.51	–
Wofacutan wash lotion	19.21	–
Abitima® clinic face cream	21.06	–
Base cream Taoasis	22.80	–
Hans Karrer Lipolotion MicroSilver	33.26	–
Hans Karrer Lipocream MicroSilver	34.44	–

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Substanz	Distance in main model	Distance in second-stage model
Asche Basis® lotion	35.82	–
Fenistil® Gel	36.30	–
Neuroderm® moisturising cream	37.45	–
Neuroderm® care lotion	37.80	–
DMS® base cream classic	38.13	–
Fabitop® base cream	40.05	–
Eucerinum W/O basis	41.14	–
Excipial® U10 Lipolotio	43.55	–
DMS® base cream high classic	46.20	–
Eucerinum O/W basis	49.55	–
Neribas® cream	49.73	–

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

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	11.37
31073	31073	0.00	11.03
31279	31279	0.00	10.90
31495	31495	0.00	21.02
31509	31509	0.00	31.47
31536	31536	0.00	11.19
31628	31628	0.00	31.25
31958	31958	0.00	22.06
33502	33502	0.00	33.35
33789	33789	0.00	20.66
35469	35469	0.00	10.29
36764	36764	0.00	33.58
36768	36768	0.00	7.73

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Lygal® head ointment N 3%**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	10005426-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lygal® head ointment N 3%

Special notes

When selecting the *Lygal® head ointment N 3%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Lygal® head ointment N 3%	3	2	12

Second-stage model

For differentiation of the substance/substance group *Lygal® head ointment N 3%* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Lygal® head ointment N 3%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Almirall	Lygal® head ointment N 3%	222212	36765	40	not required
Taurus	Lygal® head ointment N 3%	124311	31049	40	not required
Taurus	Lygal® head ointment N 3%	143710	31763	60	not required

Validation samples

A total of 70 089 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 *Lygal® head ointment N 3%*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Lygal® head ointment N 3%*.
- 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
Taurus	Lygal® head ointment N 3%	160732	32763	40
Taurus	Lygal® head ointment N 3%	181802	34127	40
Taurus	Lygal® head ointment N 3%	160732	33261	40

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- 25 981 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 7 *Apo-Ident* customers from 12 batches from the substance/substance group *Lygal® head ointment N 3%*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Almirall Hermal/Noweda	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
Almirall	Lygal® head ointment N 3%	174928	1
Almirall	Lygal® head ointment N 3%	181908	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
Taurus Pharma	Lygal® head ointment N 3%	134507	1

- 15 420 spectra from 1165 *Apo-Ident* customers from a total of 5012 batches from a further 158 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 *Lygal® head ointment N 3%* 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 *Lygal® head ointment N 3%* 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	28 415
Type B	0	120	0	25 981
Type C	0	13	0	15 420

The substance/substance group *Lygal® head ointment N 3%* 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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9688 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Lygal® head ointment N 3%* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Lygal® ointment base	18.35	–
Stomahesive® adhesive paste	54.30	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lygal® head ointment N 3%* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

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
31049	31049	0.00	38.80
31763	31763	0.00	38.98
36765	36765	0.00	35.97

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Lygal® ointment base**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31014-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lygal® ointment base

Special notes

When selecting the *Lygal® ointment base* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Lygal® ointment base	4	2	34

Second-stage model

For differentiation of the substance/substance group *Lygal®* *ointment base* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Lygal®* *ointment base*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Almirall	Lygal® ointment base	222801	36892	40	not required
Taurus	Lygal® ointment base	121302P	31014	40	not required
Taurus	Lygal® ointment base	154841	32749	40	not required
Taurus	Lygal® ointment base	164201	32772	40	not required
Taurus	Lygal® ointment base	164201	33244	40	not required
Taurus	Lygal® ointment base	164201	33297	40	not required

Validation samples

A total of 70 089 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 *Lygal®* *ointment base*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 28 315 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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.

- 100 spectra of 2 reference samples from the substance/substance group *Lygal®* *ointment base*.
- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Almirall	Lygal® ointment base	174104	33988	40
Taurus	Lygal® ointment base	124904P	31704	60

- 26 001 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 123 spectra from 51 *Apo-Ident* customers from 35 batches from the substance/substance group *Lygal® ointment base*.

- 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
Allmiral/Noweda	Lygal® ointment base	202504	2
Allmirall/Taurus	Lygal® ointment base	202503	1
Allmirall	Lygal® ointment base	202504	1
Almiral / Gehe	Lygal® ointment base	175007	4
Almiral / Gehe	Lygal® ointment base	182905	2
Almiral / Gehe	Lygal® ointment base	202503	1
Almiral/ Phönix	Lygal® ointment base	174106	1
Almiral/Anzag	Lygal® ointment base	213602	1
Almirall Hermal GmbH/No...	Lygal® ointment base	192701	1
almirall Hermal GmbH	Lygal® ointment base	192701	1
Almirall Hermal GmbH	Lygal® ointment base	202503	1
Almirall Hermal GmbH	Lygal® ointment base	202504	1
Almirall/ Gehe	Lygal® ointment base	175008	2
Almirall/ Jenne	Lygal® ointment base	202102	1
Almirall/	Lygal® ointment base	202504	1
Almirall/Fiebig	Lygal® ointment base	202503	1
almirall/gehe	Lygal® ointment base	174106	1
Almirall/GEHE	Lygal® ointment base	182903	1
Almirall/Gehe	Lygal® ointment base	182904	1
Almirall/Gehe	Lygal® ointment base	202504	3
Almirall/GE-HH	Lygal® ointment base	202503	3
Almirall/Hermal GmbH/No...	Lygal® ointment base	182904	1
Almirall/Noweda EK 8,62...	Lygal® ointment base	202504	1
Almirall/Noweda	Lygal® ointment base	175008	1
Almirall/Noweda	Lygal® ointment base	182903	1
Almirall/Noweda	Lygal® ointment base	192701	1
Almirall/Noweda	Lygal® ointment base	202504	1
Almirall/NOWEDA	Lygal® ointment base	214603	1
Almirall/Phoenix	Lygal® ointment base	182904	1
Almirall/Phoenix	Lygal® ointment base	202101	1
Almirall/Sanacorp	Lygal® ointment base	213602	1
Almirall	Lygal® ointment base	174106	2
Almirall	Lygal® ointment base	175007	2
Almirall	Lygal® ointment base	175008	1
Almirall	Lygal® ointment base	182001	5
Almirall	Lygal® ointment base	182002	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Almirall	Lygal® ointment base	182903	4
Almirall	Lygal® ointment base	182904	4
Almirall	Lygal® ointment base	184607	2
Almirall	Lygal® ointment base	192701	2
Almirall	Lygal® ointment base	193202	2
Almirall	Lygal® ointment base	202102	2
Almirall	Lygal® ointment base	202503	1
Almirall	Lygal® ointment base	202504	4
Almirall	Lygal® ointment base	211301	1
Almirall	Lygal® ointment base	213602	1
almirall	Lygal® ointment base	214603	1
Almirall	Lygal® ointment base	214603	1
Caelo	Lygal® ointment base	141601P	1
Caelo	Lygal® ointment base	154841	1
Caelo	Lygal® ointment base	174106	1
Caelo	Lygal® ointment base	182903	1
Caelo	Lygal® ointment base	202504	1
Finteler Apotheke	Lygal® ointment base	1704011	1
Gehe/ Almirall	Lygal® ointment base	182904	1
Hermal/Noweda	Lygal® ointment base	202101	2
Phoenix WE: 08.11.17 20...	Lygal® ointment base	172803_2	1
Phönix/Almirall	Lygal® ointment base	182904	1
Sanacorp/Almirall	Lygal® ointment base	175008	1
TAUROS PHARMA	Lygal® ointment base		1
TAUROS PHARMA	Lygal® ointment base	124803	1
TAUROS PHARMA	Lygal® ointment base	141601P	1
Taurus / Gehe	Lygal® ointment base	1704011	1
Taurus Pharma / Gehe	Lygal® ointment base	133401T	1
Taurus Pharma GmbH	Lygal® ointment base	164803	1
Taurus Pharma GmbH	Lygal® ointment base	172803_2	1
Taurus Pharma/Jenne	Lygal® ointment base	1728031	1
Taurus Pharma/Jenne	Lygal® ointment base	193202	2
Taurus Pharma	Lygal® ointment base	133401P	1
Taurus Pharma	Lygal® ointment base	133401T	2
Taurus Pharma	Lygal® ointment base	141601P	4
TAURUS PHARMA	Lygal® ointment base	141602T	1
TAURUS PHARMA	Lygal® ointment base	154841	1
Taurus Pharma	Lygal® ointment base	182904	1
Taurus/ Phönix	Lygal® ointment base	133401T	1
Taurus/Alliance	Lygal® ointment base	1717021	1
Taurus/Alliance	Lygal® ointment base	1717022	2
Taurus/Phönix	Lygal® ointment base	154841	1
Taurus	Lygal® ointment base	124803	2
Taurus	Lygal® ointment base	133401T	2
Taurus	Lygal® ointment base	133402	1
Taurus	Lygal® ointment base	141601T	1
Taurus	Lygal® ointment base	141603	2
Taurus	Lygal® ointment base	18121705	1

- 15 310 spectra from 1163 *Apo-Ident* customers from a total of 4989 batches from a further 158 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*.

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Validation results

The validation runs checked whether the substance/substance group *Lygal®* *ointment base* 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 *Lygal®* *ointment base* 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	28 315
Type B	0	100	0	26 001
Type C	0	123	0	15 310

The substance/substance group *Lygal®* *ointment base* 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 % (> 99.9637 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 98.9652 %)	100.0000 % (> 95.1220 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Lygal®* *ointment base* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Lygal® head ointment N 3%	16.93	–
Stomahesive® adhesive paste	38.06	–
Asche Basis® fat ointment	115.50	–

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

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
31014	31014	0.00	21.37
32749	32749	0.00	25.81
32772	32772	0.00	31.09
33244	33244	0.00	27.46
33297	33297	0.00	23.16
36892	36892	0.00	24.68

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Mandarin oil, green**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`33798-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	1

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 475 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Mandarin oil, green*.

- 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
Taoasis	Mandarin oil, green	110776-2806	1

- 15 432 spectra from 1165 *Apo-Ident* customers from a total of 5023 batches from a further 158 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	28 475
Type B	0	80	0	26 021
Type C	0	1	0	15 432

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 % (> 99.9642 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0163 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Mandarin oil, green* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Citric oil	24.55	–
Lime oil	28.90	–
Grapefruit oil, organic	36.26	–
Orange oil	48.78	–

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.

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	23.84
33806	33806	0.00	24.25

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Manuka oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31545-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	4	2	12

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Manuka oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 25 981 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 23 spectra from 4 *Apo-Ident* customers from 14 batches from the substance/substance group *Manuka oil*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Canea Pharma GmbH	Manuka oil		1
Primavera	Manuka oil	899C28	1
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	2
Taoasis	Manuka oil	65261-127051	1
Taoasis	Manuka oil	83579-2220	4
Taoasis	Manuka oil	96134-2223	1
Taoasis	Manuka oil	96134-2927	3

- 15 410 spectra from 1165 *Apo-Ident* customers from a total of 5010 batches from a further 158 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	200	0	28 355
Type B	0	120	0	25 981
Type C	0	23	0	15 410

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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9671 %)	100.0000 % (> 73.9130 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Manuka oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Vetiver bourbon oil	13.19	–
Cypress oil	33.59	–
Myrtle oil	34.93	–
Immortelle oil	36.89	–
Citus oil	40.04	–
Marjoram oil	41.96	–
Cardamom oil	44.23	–
Hyssop oil	47.48	–
Cumin oil	48.48	–
Salmon oil	53.03	–

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.

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	34.84
31655	31655	0.00	34.13
33994	33994	0.00	25.87
35075	35075	0.00	22.38

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

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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 2.5-2023-04

Validated substance/substance group	**Marjoram oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30454-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	26

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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 *Marjoram oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 28 255 spectra from a total of 597 batches from further 159 substances. These spectra were recorded by *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 by *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*.

*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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- 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

- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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 12 *Apo-Ident* customers from 26 batches from the substance/substance group *Marjoram 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
Bombastus	Marjoram oil	278279	1
Caelo	Marjoram oil	12041602	7
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
Taoasis/Gehe	Marjoram oil	29293-98717	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

- 15 394 spectra from 1165 *Apo-Ident* customers from a total of 4998 batches from a further 158 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	28 255
Type B	0	120	0	25 981
Type C	0	39	0	15 394

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 % (> 99.9636 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9661 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Marjoram oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Carrot seed oil	23.16	–
Tea tree oil	25.82	–
Patchouli oil	45.52	–
Yarrow oil	60.14	–

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.

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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	65.95
32067	32067	0.00	41.22
32819	32819	0.00	52.16
34275	34275	0.00	60.14
34436	34436	0.00	45.22
36741	36741	0.00	43.45
37665	37665	0.00	70.79

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 2.5-2023-04

Validated substance/substance group	**Matricaria oil, morrocan**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30844-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	8

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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.

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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

- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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 4 *Apo-Ident* customers from 8 batches from the substance/substance group *Matricaria oil, morrocan*.

- 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
Taoasis/Taoasis	Matricaria oil, morrocan	1814-127407	1
Taoasis/Taoasis	Matricaria oil, morrocan	2022-960	1
Taoasis/Taoasis	Matricaria oil, morrocan	5081-8452	1
Taoasis	Matricaria oil, morrocan	6159-93239	1
Taoasis	Matricaria oil, morrocan	6631-104465	1
Taoasis	Matricaria oil, morrocan	7111-12881	1
Taoasis	Matricaria oil, morrocan	711114502	1
Taoasis	Matricaria oil, morrocan	7111-14502	2

- 15 424 spectra from 1165 *Apo-Ident* customers from a total of 5016 batches from a further 158 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	28 355
Type B	0	120	0	25 981
Type C	0	7	2	15 424

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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9705 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Matricaria oil, morrocan* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, white	34.38	–
Marjoram oil	38.96	–
Citus oil	41.04	–
Angelica root oil	45.22	–
Yarrow oil	51.21	–

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.

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	41.45
31841	31841	0.00	43.15
32269	32269	0.00	51.62
37663	37663	0.00	43.85

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Matricaria oil, roman**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31254-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 25 981 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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
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

- 15 413 spectra from 1165 *Apo-Ident* customers from a total of 5014 batches from a further 158 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	28 355
Type B	0	105	15	25 981
Type C	0	20	0	15 413

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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9510 %)	87.5000 % (> 85.0000 %)
Type C	100.0000 % (> 98.9674 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Matricaria oil, roman* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Sage oil	24.50	–
Hyssop oil	33.71	–
Citus oil	33.72	–
Rosemary camphor oil	36.10	–
Spruce needle oil	37.57	–
Cedar wood oil	47.38	–
Rosemary oil	49.43	–
Cardamom oil	51.00	–

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.

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	36.00
31686	31686	0.00	37.61
33989	33989	0.00	33.71
35538	35538	0.00	24.50

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Melissa oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	33800-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	4	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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Melissa oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 28 395 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 071 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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.

- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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	160	0	28 395
Type B	0	30	0	26 071
Type C	0	0	0	15 433

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 % (> 99.9638 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9516 %)	100.0000 % (> 80.0000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Melissa oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Immortelle oil	15.35	–
Ginger oil	22.63	–
Lemon grass oil	23.66	–
Cypress oil	26.63	–
Dwarf pine oil	29.57	–
Marjoram oil	32.31	–
Spearmint oil	33.62	–
Cedar wood oil	33.67	–
Swiss pine oil	36.03	–
Citus oil	38.07	–
Myrtle oil	40.03	–
Vetiver bourbon oil	43.90	–
Citronella oil	44.02	–
Patchouli oil	44.11	–
Carrot seed oil	44.50	–
Tea tree oil	47.90	–
Silver fir oil	49.19	–
Lime oil	50.05	–

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.

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	20.74
33831	33831	0.00	20.87
34166	34166	0.00	23.66
34404	34404	0.00	17.49

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Melissa oil 30%**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`33812-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 475 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 071 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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.
- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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	28 475
Type B	0	30	0	26 071
Type C	0	0	0	15 433

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 % (> 99.9642 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9516 %)	100.0000 % (> 80.0000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Melissa oil 30%* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, white	25.85	–
Petitgrain oil	26.93	–
Neroli oil	30.57	–
Matricaria oil, morrocan	30.98	–
Lavender oil	37.40	–
Spearmint oil	47.19	–
Juniper oil	47.68	–
Yarrow oil	49.23	–

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.

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	26.93
33962	33962	0.00	28.51

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Myrrh oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30748-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	4	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

Calibration samples

Only spectra which have been recorded by *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
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

Validation samples

A total of 70 089 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 *Myrrh oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 28 375 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 25 981 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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

- 15 428 spectra from 1165 *Apo-Ident* customers from a total of 5020 batches from a further 158 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	180	0	28 375
Type B	0	80	40	25 981
Type C	0	4	1	15 428

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 % (> 99.9638 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9510 %)	66.6667 % (> 64.1667 %)
Type C	100.0000 % (> 98.9751 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Myrrh oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Orange oil	49.66	–
Grapefruit oil, organic	52.92	–

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.

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	111.68
32271	32271	0.00	155.01
33992	33992	0.00	44.22
37667	37667	0.00	146.90

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Neroli oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	31260-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	5	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

Calibration samples

Only spectra which have been recorded by *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
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 70 089 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 *Neroli oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 28 335 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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.

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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

- 25 941 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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.
- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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	220	0	28 335
Type B	0	80	80	25 941
Type C	0	0	0	15 433

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 % (> 99.9637 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9509 %)	50.0000 % (> 48.1250 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Neroli oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, white	22.46	–
Matricaria oil, morrocan	25.68	–
Lavender oil	31.68	–
Basil oil	39.26	–
Coriander oil	49.47	–
Melissa oil 30%	51.77	–

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.

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	48.06
31695	31695	0.00	53.66
34283	34283	0.00	56.84
34406	34406	0.00	41.65
37668	37668	0.00	39.26

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Neuroderm® moisturising cream lipo**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30721-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Neuroderm® moisturising cream lipo

Special notes

When selecting the *Neuroderm® moisturising cream lipo* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Neuroderm® moisturising cream lipo	5	3	1

Second-stage model

For differentiation of the substance/substance group *Neuroderm® moisturising cream lipo* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Neuroderm® moisturising cream lipo*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Infectopharm	Neuroderm® moisturising crea…	S031202.1	30721	40	not required
Infectopharm	Neuroderm® moisturising crea…	S031506.1	31672	60	not required
Infectopharm	Neuroderm® moisturising crea…	S051723.1	34045	40	not required
Infectopharm	Neuroderm® moisturising crea…	S072214.1	37417	30	not required
Infectopharm	Neuroderm® moisturising crea…	S082224.1	37453	30	not required

Validation samples

A total of 70 089 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 *Neuroderm® moisturising cream lipo*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 28 355 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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 *Neuroderm® moisturising cream lipo*.

- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Infectopharm	Neuroderm® moisturising crea…	S071617.2	32739	40
Infectopharm	Neuroderm® moisturising crea…	S021706.1	33287	40
Infectopharm	Neuroderm® moisturising crea…	S022106.1	36607	40

- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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 *Neuroderm® moisturising cream lipo*.
- 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.

Supplier	Substance	Batch	Spectra
Infectopharm/AHD	Neuroderm® moisturising crea…		1
Infectopharm	Neuroderm® moisturising crea…		1

- 15 431 spectra from 1165 *Apo-Ident* customers from a total of 5023 batches from a further 158 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 *Neuroderm® moisturising cream lipo* 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 *Neuroderm® moisturising cream lipo* 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	28 355
Type B	0	120	0	25 981
Type C	0	2	0	15 431

The substance/substance group *Neuroderm® moisturising cream lipo* 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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9905 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Neuroderm® moisturising cream lipo* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
ALLERGIKA®-Lipolotio urea 5% F	15.23	–
Dermatest base ointment	21.87	–
Excipial® U Lipolotio	52.40	–

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

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
30721	30721	0.00	30.62
31672	31672	0.00	23.97
34045	34045	0.00	30.71
37417	37417	0.00	31.00
37453	37453	0.00	29.45

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Nicotine**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31019-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 370 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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.

- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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	28 370
Type B	0	40	0	26 061
Type C	0	0	0	15 433

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 % (> 99.9638 %)	100.0000 % (> 96.7568 %)
Type B	100.0000 % (> 99.9514 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Nicotine* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Dichloroacetic acid	146.87	–

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.

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	161.52
31508	31508	0.00	160.30
31518	31518	0.00	160.60
31948	31948	0.00	161.06

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Ointment ash basis / Neribas®**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30774-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ointment ash basis / Neribas®; Asche Basis® ointment; Neribas® ointment

Special notes

When selecting the *Ointment ash basis / Neribas®* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Ointment ash basis / Neribas®	5	5	137

Second-stage model

For differentiation of the substance/substance group *Ointment ash basis / Neribas®* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Ointment ash basis / Neribas®*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Chiesi	Asche Basis® ointment	21038A	30774	40	not required
Chiesi	Asche Basis® ointment	21038A	30833	40	not required
Chiesi	Asche Basis® ointment	21038A	31080	40	not required
Chiesi	Asche Basis® ointment	13004A	36763	40	not required
Bayer	Neribas® ointment	21053B	30969	40	not required
Bayer	Neribas® ointment	21053B	30994	40	not required
Jenapharm	Neribas® ointment	31064C	31093	40	not required
Karo Pharma G…	Neribas® ointment	YY04T3L	35480	40	not required

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 8 reference samples from the substance/substance group *Ointment ash basis / Neribas®*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 28 235 spectra from a total of 599 batches from further 158 substances. These spectra were recorded by *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 by *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.

- 280 spectra of 7 reference samples from the substance/substance group *Ointment ash basis / Neribas®*.
- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Chiesi	Asche Basis® ointment	61067A	32590	40
Chiesi	Asche Basis® ointment	17072A	33840	40
Chiesi	Asche Basis® ointment	02089A	35457	40
Jenapharm	Neribas® ointment	YY00TJ0	32564	40
Jenapharm	Neribas® ointment	YY016EC	33288	40
Chiesi	Asche Basis® ointment	61067A	32924	40
Chiesi	Asche Basis® ointment	61067A	32927	40

- 25 821 spectra from a total of 583 batches from further 208 substances. These spectra were recorded by *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.

- 426 spectra from 94 *Apo-Ident* customers from 141 batches from the substance/substance group *Ointment ash basis / Neribas®*.

- Among them are spectra of independent samples from 135 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Alliance Healthcare	Asche Basis® ointment	92083A	1
Anzag/Ichtyol-Gesellsch...	Asche Basis® ointment	23043A	1
Audor Pharma	Neribas® ointment	YY02825	1
Bayer/ Sanacorp	Neribas® ointment	YY006JT	3
Bayer/Sanacorp	Neribas® ointment	YY00THL	1
Bayer	Neribas® ointment	YY01KHH	1
Caelo	Asche Basis® ointment	31047A	1
Caelo	Asche Basis® ointment	61067A	1
Caelo	Asche Basis® ointment	63068A	3
Caelo	Asche Basis® ointment	81708A	1
Caelo	Asche Basis® ointment	83079A	2
Caelo	Asche Basis® ointment	83080A	1
Caelo	Asche Basis® ointment	94087A	1
Caelo	Neribas® ointment	YY00CC8	1
Caelo	Neribas® ointment	YY00THL	2
Caelo	Neribas® ointment	YY00TJ0	1
Caelo	Neribas® ointment	YY00XEH	1
Caelo	Neribas® ointment	YY016EC	1
Caelo	Neribas® ointment	YY016LN	1
Chiese/Sanacorp WE:07.0...	Asche Basis® ointment	52062A	1
Chiese	Asche Basis® ointment	63069A	1
Chiese	Asche Basis® ointment	63070A	1
Chiese	Asche Basis® ointment	71073A	2
Chiesi / Gehe	Asche Basis® ointment	33049A	1
Chiesi / Gehe	Asche Basis® ointment	33050A	1
Chiesi / Jenne	Asche Basis® ointment	11002A	1
Chiesi / Jenne	Asche Basis® ointment	12003A	1
Chiesi / Jenne	Asche Basis® ointment	2088A	1
Chiesi / Jenne	Asche Basis® ointment	94087A	1
Chiesi / Noweda	Asche Basis® ointment	2088A	3
Chiesi / Noweda	Asche Basis® ointment	3090A	1

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Supplier	Substance	Batch	Spectra
Chiesi / Phönix	Asche Basis® ointment	2089A	1
Chiesi / Phönix	Asche Basis® ointment	83079A	1
Chiesi / Phönix	Asche Basis® ointment	83080A	1
Chiesi / Phönix	Asche Basis® ointment	91082A	3
Chiesi / Phönix	Asche Basis® ointment	92083A	1
Chiesi / Phönix	Asche Basis® ointment	92084A	2
Chiesi / Phönix	Asche Basis® ointment	92086A	1
Chiesi / Phönix	Asche Basis® ointment	92087A	1
Chiesi / Phönix	Asche Basis® ointment	94087A	1
Chiesi / Sanacorp	Asche Basis® ointment	92084A	1
Chiesi / Sanacorp	Asche Basis® ointment	92086A	1
chiesi /Gehe	Asche Basis® ointment	73075A	1
Chiesi /Jenne	Asche Basis® ointment	92437A	1
Chiesi GmbH / AHD	Asche Basis® ointment	22010A	1
Chiesi GmbH / Sanacorp	Asche Basis® ointment	12003A	1
Chiesi GmbH / Sanacorp	Asche Basis® ointment	14006A	1
Chiesi GmbH / Sanacorp	Asche Basis® ointment	21008A	1
Chiesi GmbH / Sanacorp	Asche Basis® ointment	92034A	1
Chiesi GmbH/ Allianz He...	Asche Basis® ointment	13005A	1
Chiesi GmbH/ Gehe	Asche Basis® ointment	12003A	1
Chiesi GmbH/ Gehe	Asche Basis® ointment	13005A	1
Chiesi GmbH/ Phoenix	Asche Basis® ointment	3090A	1
Chiesi GmbH/Phoenix	Asche Basis® ointment	2089A	2
Chiesi GmbH/Phoenix	Asche Basis® ointment	83080A	1
Chiesi GmbH/Phoenix	Asche Basis® ointment	91082A	1
Chiesi GmbH/Phoenix	Asche Basis® ointment	92083A	3
Chiesi GmbH	Asche Basis® ointment	2089A	1
Chiesi Gmbh	Asche Basis® ointment	21039A	1
Chiesi GmbH	Asche Basis® ointment	52062A	1
Chiesi GmbH	Asche Basis® ointment	52063A	3
Chiesi GmbH	Asche Basis® ointment	52064A	3
Chiesi GmbH	Asche Basis® ointment	53065A	4
Chiesi GmbH	Asche Basis® ointment	61066A	2
Chiesi GmbH	Asche Basis® ointment	63070A	2
Chiesi GmbH	Asche Basis® ointment	71071A	1
Chiesi GmbH	Asche Basis® ointment	71072A	1
Chiesi GmbH	Asche Basis® ointment	71073A	1
Chiesi GmbH	Asche Basis® ointment	72074A	1
Chiesi GmbH	Asche Basis® ointment	84081A	1
Chiesi GmbH	Asche Basis® ointment	91082A	1
Chiesi GmbH	Asche Basis® ointment	92083A	3
Chiesi GmbH	Asche Basis® ointment	92084A	1
Chiesi GmbH	Asche Basis® ointment	92086A	1
Chiesi/ Anzag	Asche Basis® ointment	3090A	1
Chiesi/ Anzag	Asche Basis® ointment	83079A	1
Chiesi/ Gehe	Asche Basis® ointment	11002A	1
Chiesi/ Gehe	Asche Basis® ointment	2088A	1
Chiesi/ Jenne	Asche Basis® ointment	21007A	4
Chiesi/ Noweda EK 5,70	Asche Basis® ointment	2001A	1
CHIESI/ NOWEDA	Asche Basis® ointment	51060A	2
Chiesi/ Phenix	Asche Basis® ointment	92085A	1
Chiesi/ Phoenix	Asche Basis® ointment	2089A	1
Chiesi/ Phoenix	Asche Basis® ointment	92083A	1
Chiesi/ Sanacorp	Asche Basis® ointment	92085A	1
Chiesi/ sanacorp	Asche Basis® ointment	92086A	1
Chiesi/AHD	Asche Basis® ointment	14006A	2
Chiesi/AHD	Asche Basis® ointment	31045A	4
Chiesi/AHD	Asche Basis® ointment	31047A	1
Chiesi/AHD	Asche Basis® ointment	33049A	1
Chiesi/Alliance	Asche Basis® ointment	61067A	1

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Supplier	Substance	Batch	Spectra
Chiesi/Anzag	Asche Basis® ointment	1(92084A)	1
Chiesi/Anzag	Asche Basis® ointment	11002A	4
Chiesi/Anzag	Asche Basis® ointment	2001A	1
Chiesi/anzag	Asche Basis® ointment	21007A	1
Chiesi/Anzag	Asche Basis® ointment	3090A	1
Chiesi/Gehe	Asche Basis® ointment	11002A	4
Chiesi/Gehe	Asche Basis® ointment	12003A	2
Chiesi/Gehe	Asche Basis® ointment	2001A	1
Chiesi/Gehe	Asche Basis® ointment	2088A	1
Chiesi/Gehe	Asche Basis® ointment	2089A	1
Chiesi/Gehe	Asche Basis® ointment	3090A	2
Chiesi/Gehe	Asche Basis® ointment	42056A	1
chiesi/gehe	Asche Basis® ointment	71072A	1
Chiesi/Gehe	Asche Basis® ointment	83079A	1
Chiesi/Gehe	Asche Basis® ointment	92085A	2
Chiesi/Gehe	Asche Basis® ointment	94087A	1
Chiesi/Jenne	Asche Basis® ointment		1
Chiesi/Jenne	Asche Basis® ointment	13005A	3
Chiesi/Jenne	Asche Basis® ointment	2001A	1
Chiesi/Jenne	Asche Basis® ointment	73076A	1
Chiesi/Jenne	Asche Basis® ointment	74077A	2
Chiesi/Jenne	Asche Basis® ointment	91082A	2
Chiesi/Jenne	Asche Basis® ointment	92083A	5
Chiesi/Jenne	Asche Basis® ointment	92084A	1
Chiesi/Jenne	Asche Basis® ointment	92086A	2
Chiesi/Jenne	Asche Basis® ointment	925084A	1
Chiesi/Krieger	Asche Basis® ointment	61066A	1
Chiesi/Noweda	Asche Basis® ointment	11002A	2
Chiesi/Noweda	Asche Basis® ointment	12003A	1
Chiesi/Noweda	Asche Basis® ointment	2089A	1
Chiesi/Noweda	Asche Basis® ointment	71072A	1
Chiesi/Noweda	Asche Basis® ointment	83080A	1
Chiesi/Phoenix	Asche Basis® ointment	2089A	1
Chiesi/Phoenix	Asche Basis® ointment	21007A	1
Chiesi/Phoenix	Asche Basis® ointment	23042A	1
Chiesi/Phoenix	Asche Basis® ointment	3090A	1
Chiesi/Phoenix	Asche Basis® ointment	73075A	3
Chiesi/Phoenix	Asche Basis® ointment	73076A	1
Chiesi/Phoenix	Asche Basis® ointment	74077A	1
Chiesi/Phoenix	Asche Basis® ointment	83079A	1
Chiesi/Phoenix	Asche Basis® ointment	84081A	3
Chiesi/Phoenix	Asche Basis® ointment	91082A	2
Chiesi/Phoenix	Asche Basis® ointment	92083A	1
Chiesi/Phoenix	Asche Basis® ointment	92084A	3
Chiesi/Phoenix	Asche Basis® ointment	92086A	2
Chiesi/Phoenix	Asche Basis® ointment	94087A	1
Chiesi/Phönix	Asche Basis® ointment	2088A	1
Chiesi/Phönix	Asche Basis® ointment	3090A	2
Chiesi/Phönix	Asche Basis® ointment	51059A	1
Chiesi/Phönix	Asche Basis® ointment	71073A	1
Chiesi/Phönix	Asche Basis® ointment	72074A	2
Chiesi/Phönix	Asche Basis® ointment	81078A	1
Chiesi/Phönix	Asche Basis® ointment	84081A	2
Chiesi/Sanacorp	Asche Basis® ointment	41053A	1
Chiesi/Sanacorp	Asche Basis® ointment	71072A	1
Chiesi/Sanacorp	Asche Basis® ointment	83080A	1
Chiesi/Sanacorp	Asche Basis® ointment	92084A	1
Chiesi	Asche Basis® ointment	14006A	1
Chiesi	Asche Basis® ointment	2089A	1
Chiesi	Asche Basis® ointment	21008A	1

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Supplier	Substance	Batch	Spectra
Chiesi	Asche Basis® ointment	32048A	1
Chiesi	Asche Basis® ointment	33049A	1
Chiesi	Asche Basis® ointment	34051A	1
Chiesi	Asche Basis® ointment	41052A	1
Chiesi	Asche Basis® ointment	41054A	3
chiesi	Asche Basis® ointment	42055A	1
chiesi	Asche Basis® ointment	44057A	1
Chiesi	Asche Basis® ointment	510604	1
Chiesi	Asche Basis® ointment	51060A	1
Chiesi	Asche Basis® ointment	52062A	3
Chiesi	Asche Basis® ointment	52063A	1
Chiesi	Asche Basis® ointment	53065A	2
Chiesi	Asche Basis® ointment	63068A	1
Chiesi	Asche Basis® ointment	63069A	3
Chiesi	Asche Basis® ointment	83079A	3
Chiesi	Asche Basis® ointment	83080A	1
Chiesi	Asche Basis® ointment	94087A	1
Chieso	Asche Basis® ointment	52063A	2
Chisie/Jenne	Asche Basis® ointment	12003A	1
Dr. Wolff	Neribas® ointment	YY00THL	2
Fa. Chiesi/NOweda	Asche Basis® ointment	91082A	1
Gehe	Asche Basis® ointment	17I21-B01	1
Gehe	Asche Basis® ointment	83080A	2
Gehe	Neribas® ointment	YY023JE	1
GP Grenzach Produktions...	Neribas® ointment	YY01FX4	1
Jenaparm	Neribas® ointment	12091812	1
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	YY00THL	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 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	YY00K7E	2
Jenapharm/ Gehe	Neribas® ointment	YY01TF3	2
Jenapharm/ Gehe	Neribas® ointment	YY023J1	1
Jenapharm/ Gehe	Neribas® ointment	YY02825	3
Jenapharm/ Gehe	Neribas® ointment	YY02L27	2
Jenapharm/ Gehe	Neribas® ointment	YY02L88	1
Jenapharm/ Sanacorp	Neribas® ointment	YY00THL	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	1
Jenapharm/Anzag	Neribas® ointment	69(YY01YEX)	1

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Supplier	Substance	Batch	Spectra
Jenapharm/Anzag	Neribas® ointment	YY00XEH	2
Jenapharm/Gehe	Neribas® ointment	YY01FX4	1
Jenapharm/Gehe	Neribas® ointment	YY01YEX	1
Jenapharm/Gehe	Neribas® ointment	YY023JE	1
Jenapharm/Gehe	Neribas® ointment	YY02L88	1
Jenapharm/Jenne	Neribas® ointment	61(YY019PE)	1
Jenapharm/Jenne	Neribas® ointment	YY01TF3	1
Jenapharm/Jenne	Neribas® ointment	YY04F1P	1
Jenapharm/Noweda	Neribas® ointment	YY00THL	1
Jenapharm/Phoenix	Neribas® ointment	YY023JE	1
Jenapharm/Phönix	Neribas® ointment	YY006JT	1
Jenapharm/Phönix	Neribas® ointment	YY01KHH	1
Jenapharm/Sanacorp	Neribas® ointment	YY0180C	1
Jenapharm	Neribas® ointment	5121811	1
Jenapharm	Neribas® ointment	YY006JT	1
Jenapharm	Neribas® ointment	YY00K7E	1
Jenapharm	Neribas® ointment	YY00TJ0	1
Jenapharm	Neribas® ointment	YY00XEH	1
Jenapharm	Neribas® ointment	YY011KX	1
Jenapharm	Neribas® ointment	YY016EC	1
Jenapharm	Neribas® ointment	YY016LN	2
Jenapharm	Neribas® ointment	YY017LF	1
Jenapharm	Neribas® ointment	YY01FX4	4
Jenapharm	Neribas® ointment	YY01KHH	2
Jenapharm	Neribas® ointment	YY01TF3	2
Jenapharm	Neribas® ointment	YY023J1	1
Jenapharm	Neribas® ointment	YY023JE	3
Jenapharm	Neribas® ointment	YY02825	7
Jenapharm	Neribas® ointment	YY02L88	4
JenapharmGmbH/Sanacorp	Neribas® ointment	YY02L88	2
Jenne/Chiesi	Asche Basis® ointment	21008A	1
Jenne	Neribas® ointment	YY0577C	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(YY04T3L)	1
Karo Pharma / Anzag	Neribas® ointment	220323(YY051T5)	1
Karo Pharma / Anzag	Neribas® ointment	220323(YY051T6)	1
Karo Pharma / Anzag	Neribas® ointment	220721(YY0577C)	1
Karo Pharma / Anzag	Neribas® ointment	99(YY04F1P)	1
Karo Pharma / Jenne	Neribas® ointment	220518(YY0577C)	1
Karo Pharma / Jenne	Neribas® ointment	98(YY04F1P)	1
Karo Pharma AB/ Noweda/...	Neribas® ointment	YY04F1P	1
KARO Pharma/ GEHE	Neribas® ointment	YY051T5	1
KARO Pharma/Gehe	Neribas® ointment	YY051T5	2
Karo Pharma/Sanacorp	Neribas® ointment	YY051T5	1
Karo Pharma	Neribas® ointment	YY04F1P	1
Karo Pharma	Neribas® ointment	YY04T3L	1
Karo Pharma	Neribas® ointment	YY051T6	1
Karo/ Jenne	Neribas® ointment	YY051T5	3
Karo/Jenne	Neribas® ointment	YY051t5	1
Karo	Neribas® ointment	YY04KYC	1
Karopharma	Neribas® ointment	YY051T5	1
Leo Pharma A/S	Neribas® ointment	YY0431Y	1
Leo Pharma/ Gehe	Neribas® ointment	YY04KYC	4
Leo Pharma/ Jenne	Neribas® ointment	97(YY0431Y)	1

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Supplier	Substance	Batch	Spectra
LEO Pharma/Gehe	Neribas® ointment	YY0431Y	1
Leo/ Jenne	Neribas® ointment	YY04T3L	2
LeoPharm/Alliance	Neribas® ointment	YY01FX4	1
Leopharma/Jenne	Neribas® ointment	YY02L88	3
Noweda/Karo	Neribas® ointment	YY0577C	2
Noweda	Asche Basis® ointment	2088A	1
Noweda	Asche Basis® ointment	2089A	2
Noweda	Asche Basis® ointment	71072A	1
Noweda	Asche Basis® ointment	83080A	1
Noweda	Asche Basis® ointment	84081A	2
Noweda	Asche Basis® ointment	92085A	1
Phoenix / Karo Pharma	Neribas® ointment	yy04Kyc	1
Phoenix/Chiesi	Asche Basis® ointment	2088A	2
Phönix/ Chiesi	Asche Basis® ointment	83080A	1
Phönix/ Chiesi	Asche Basis® ointment	92083A	1
Phönix	Neribas® ointment		1
Phönix	Asche Basis® ointment	31047A	1
Phönix	Neribas® ointment	YY0431x	1
Phönix	Neribas® ointment	YY0431X	1
Phönix	Neribas® ointment	YY0431Y	1
Phönix	Neribas® ointment	YY04F1P	2
Phönix	Neribas® ointment	YY04T3L	1
PPL	Asche Basis® ointment	61067A	1
PPL	Asche Basis® ointment	71072A	2
PPL	Asche Basis® ointment	73075A	1
Römer/apo	Neribas® ointment	YY008RJ	1
Sanacorp Ulm	Asche Basis® ointment	84081A	1
Sanacorp WE 29.04.17 -8...	Asche Basis® ointment	63070A	1
Sanacorp/Chiesi WE:31.0...	Asche Basis® ointment	41054A	1
SanacorpWE:9.12.2016 ...	Asche Basis® ointment	63068A	1
WE:27.02.2016 Sanacor...	Asche Basis® ointment	52063A	1
WE:Sanacorp19.01.2016 ...	Asche Basis® ointment	52064A	2
WE14.12.16 Chiesi/Sanac...	Asche Basis® ointment	61067A	2
Wolf Apotheke	Neribas® ointment	73(YY02825)	1
Wolf Apotheke	Neribas® ointment	74(YY02825)	1
Wolff/AHD	Asche Basis® ointment	32048A	2

- 15 007 spectra from 1164 *Apo-Ident* customers from a total of 4888 batches from a further 157 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 *Ointment ash basis / Neribas®* 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 *Ointment ash basis / Neribas®* 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	320	0	28 235
Type B	0	273	7	25 741
Type C	0	413	13	15 007

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The substance/substance group *Ointment ash basis / Neribas®* 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 % (> 99.9636 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9508 %)	97.5000 % (> 96.4286 %)
Type C	100.0000 % (> 98.9649 %)	96.9484 % (> 96.2441 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Ointment ash basis / Neribas®* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Bepanthen® Wund- und Heilsalbe	19.95	–
Alfason Basis Cresa®	26.27	–
Alfason® Repair	65.18	–

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

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
30774	30774	0.00	35.06
30833	30833	0.00	36.73
30969	30969	0.00	39.42
30994	30994	0.00	35.92
31080	31080	0.00	34.25
31093	31093	0.00	31.61
35480	35480	0.00	38.20
36763	36763	0.00	27.32

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Orange aroma**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31190-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	6	7	93

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Orange aroma*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 28 295 spectra from a total of 598 batches from further 159 substances. These spectra were recorded by *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 by *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.

- 280 spectra of 7 reference samples from the substance/substance group *Orange aroma*.

*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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- Among them are spectra of independent samples from 7 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

- 25 821 spectra from a total of 581 batches from further 209 substances. These spectra were recorded by *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.

- 542 spectra from 310 *Apo-Ident* customers from 96 batches from the substance/substance group *Orange aroma*.

- Among them are spectra of independent samples from 93 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	22001814005	1
	Orange aroma	22001814010	1
	Orange aroma	22003369008	2
	Orange aroma	22003737006	1
7,95	Orange aroma	22001814010	1
Allergika/Kehr	Orange aroma	16056107	1
Audor Pharma	Orange aroma	15215409	1
Bombastus	Orange aroma	21002295004	1
Caelo	Orange aroma		1
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	1
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

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Supplier	Substance	Batch	Spectra
Caelo	Orange aroma	15215410	1
Caelo	Orange aroma	16056105	10
Caelo	Orange aroma	16056107	5
Caelo	Orange aroma	16056108	1
Caelo	Orange aroma	160566107	1
Caelo	Orange aroma	16206301	3
Caelo	Orange aroma	16206302	1
Caelo	Orange aroma	16347005	11
Caelo	Orange aroma	16347012	3
Caelo	Orange aroma	17055103	3
Caelo	Orange aroma	17055104	2
Caelo	Orange aroma	17055110	1
Caelo	Orange aroma	17300501	11
Caelo	Orange aroma	17300507	11
Caelo	Orange aroma	17300508	1
Caelo	Orange aroma	17300509	7
Caelo	Orange aroma	180830103	1
Caelo	Orange aroma	18083103	10
Caelo	Orange aroma	18205701	16
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	12
Caelo	Orange aroma	19093302	2
Caelo	Orange aroma	19093307	6
Caelo	Orange aroma	19093309	1
Caelo	Orange aroma	19093311	12
Caelo	Orange aroma	19093312	4
Caelo	Orange aroma	192968003	15
Caelo	Orange aroma	192968005	4
Caelo	Orange aroma	200000419003	1
Caelo	Orange aroma	200000419004	1
Caelo	Orange aroma	20000419003	9
Caelo	Orange aroma	20000419006	17
Caelo	Orange aroma	20000419010	2
Caelo	Orange aroma	20000419012	8
Caelo	Orange aroma	20003349001	2
Caelo	Orange aroma	20003349002	8
Caelo	Orange aroma	20003349005	16
Caelo	Orange aroma	20003349008	2
Caelo	Orange aroma	20003349011	11
Caelo	Orange aroma	2000419003	1
Caelo	Orange aroma	2000419006	1
Caelo	Orange aroma	21002295004	7
Caelo	Orange aroma	21002295010	10
Caelo	Orange aroma	21002295013	8
Caelo	Orange aroma	210022955004	1
Caelo	Orange aroma	22000874003	9
Caelo	Orange aroma	22000874008	2
Caelo	Orange aroma	22001814006	4
Caelo	Orange aroma	22001814008	3
Caelo	Orange aroma	22001814010	2
Caelo	Orange aroma	220905(22000874003)	1
Caelo	Orange aroma	23051201	1
Caelo	Orange aroma	25031304	1
Caelo	Orange aroma	4(20000419006)	1

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Supplier	Substance	Batch	Spectra
Caelo	Orange aroma	7055210022954	1
Caelo	Orange aroma	92968005	1
Caesa / Alliance Health...	Orange aroma	20003349011	1
Caesar & Loretz GmbH / ...	Orange aroma	16347005	1
Caesar & Loretz GmbH / ...	Orange aroma	21002295004	1
Caesar & Loretz GmbH / ...	Orange aroma	20003349005	1
Caesar & Loretz GmbH/ N...	Orange aroma	20000419012	1
Caesar & Loretz GmbH/ P...	Orange aroma	19093311	1
Caesar & Loretz GmbH/ S...	Orange aroma	20003349011	1
Caesar & Loretz GmbH/AHD	Orange aroma	22000874003	1
Caesar & Loretz GmbH/An...	Orange aroma	20003349011	1
Caesar & Loretz GmbH/E	Orange aroma	22000874003	2
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/No...	Orange aroma	22000874003	2
Caesar & Loretz GmbH/Ph...	Orange aroma	21002295010	1
Caesar & Loretz GmbH/Sa...	Orange aroma	20000419003	1
Caesar & Loretz GmbH/Sa...	Orange aroma	20000419006	1
Caesar & Loretz GmbH/Sa...	Orange aroma	21002295010	1
Caesar & Loretz GmbH/Sa...	Orange aroma	22000874003	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	11
Caesar & Loretz GmbH	Orange aroma	20000419006	4
Caesar & Loretz GmbH	Orange aroma	20000419007	2
Caesar & Loretz GmbH	Orange aroma	20000419012	6
Caesar & Loretz GmbH	Orange aroma	20003349001	3
Caesar & Loretz GmbH	Orange aroma	20003349002	3
Caesar & Loretz GmbH	Orange aroma	20003349005	1
Caesar & Loretz GmbH	Orange aroma	20003349011	2
Caesar & Loretz GmbH	Orange aroma	21002295004	5
Caesar & Loretz GmbH	Orange aroma	21002295010	4
Caesar & Loretz GmbH	Orange aroma	21002295013	3
Caesar & Loretz GmbH	Orange aroma	22000874003	3
Caesar & Loretz GmbH	Orange aroma	22001814006	2
Caesar & Loretz Hilden/...	Orange aroma	2003349002	1
Caesar & Loretz/Geilenk...	Orange aroma	18326103	1
Caesar & Loretz/Geilenk...	Orange aroma	20000419006	1
Caesar Loretz	Orange aroma	20000419006	1
Caesar&Lorenz	Orange aroma	21002295004	1
Caesar&Loretz GmbH/ San...	Orange aroma	17300501	1
Caesar&Loretz GmbH/ San...	Orange aroma	19093301	1
Euro OTC	Orange aroma	17055103	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

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Supplier	Substance	Batch	Spectra
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
Geilenkirchen	Orange aroma	19093301	1
Henry LamotteOlis GmbH	Orange aroma	18205701	1
Nachprüfung	Orange aroma	19093311	1
Noweda	Orange aroma	18326103	1
Noweda	Orange aroma	21002295004	1
Noweda	Orange aroma	2200874008	1
Phoenix	Orange aroma	17300509	3
Phoenix	Orange aroma	18326103	2
Phönix 17.1.19	Orange aroma	18083103	1
Phönix	Orange aroma	18083103	1
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

- 14 891 spectra from 1143 *Apo-Ident* customers from a total of 4929 batches from a further 158 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	260	0	28 295
Type B	0	280	0	25 821
Type C	0	539	3	14 891

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 % (> 99.9637 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9508 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 98.9649 %)	99.4465 % (> 98.8930 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Orange aroma* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Ethanol 70%	35.87	–
Raspberry aroma	94.41	–

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.

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	62.64
31402	31402	0.00	62.61
31510	31510	0.00	108.92
33100	33100	0.00	65.27
35087	35087	0.00	103.61
35255	35255	0.00	55.00

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Oregano oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31554-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	5	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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Oregano oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 28 315 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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.

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Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Oregano oil	43878A-123201	32939	40

- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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/ Phönix	Oregano oil	44314A-1600	1
Taoasis/Gehe	Oregano oil	6553TR-L03	1
Taoasis/Noweda	Oregano oil	B3253-16203	1
Taoasis	Oregano oil	B3010-11908	1
Taoasis	Oregano oil	B3010-13379	2
Taoasis	Oregano oil	B3253-15017	1

- 15 426 spectra from 1165 *Apo-Ident* customers from a total of 5018 batches from a further 158 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	240	0	28 315
Type B	0	40	0	26 061
Type C	0	7	0	15 426

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 % (> 99.9637 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9514 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.9722 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Oregano oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, red	26.28	–
Savory herb	65.16	–

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.

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	64.98
31779	31779	0.00	90.08
32769	32769	0.00	43.68
33649	33649	0.00	45.17
34368	34368	0.00	73.41

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Palmarosa oil, organic**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30597-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	7

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Palmarosa oil, organic*.
- 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	Palmarosa oil, organic	00500L26	34366	40
Taoasis	Palmarosa oil, organic	17524-105015BAG90451	30597	40
Taoasis	Palmarosa oil, organic	104704-129227	33856	40

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Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Palmarosa oil, organic	17524-105015BAG90451	30671	40
Taoasis	Palmarosa oil, organic	4941003-126708	33044	40

- 25 901 spectra from a total of 584 batches from further 209 substances. These spectra were recorded by *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 7 *Apo-Ident* customers from 7 batches from the substance/substance group *Palmarosa oil, organic*.

- 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
Primavera	Palmarosa oil, organic	724G27	1
Taoasis GmbH/ Taoasis	Palmarosa oil, organic	2587-7434	1
Taoasis/Sanacorp/05.08....	Palmarosa oil, organic	18545044-12851	1
Taoasis/Taoasis	Palmarosa oil, organic	121018-111872	1
Taoasis/Taoasis	Palmarosa oil, organic	2215-5590	1
Taoasis	Palmarosa oil, organic	121018-111094	1
Taoasis	Palmarosa oil, organic	121018-111872	2
Taoasis	Palmarosa oil, organic	2242	1

- 15 424 spectra from 1165 *Apo-Ident* customers from a total of 5017 batches from a further 158 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	28 415
Type B	0	200	0	25 901
Type C	0	9	0	15 424

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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 98.9705 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Palmarosa oil, organic* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Carrot seed oil	98.03	–

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.

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	119.70
33043	33043	0.00	103.86
34289	34289	0.00	112.47

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Panthenol ointment Lichtenstein**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30727-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Panthenol ointment Lichtenstein

Special notes

When selecting the *Panthenol ointment Lichtenstein* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Panthenol ointment Lichtenstein	3	2	0

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Panthenol ointment Lichtenstein*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Winthrop	Panthenol ointment Lichtenst…	2290680H	30727	40	not required
Winthrop	Panthenol ointment Lichtenst…	2290718H	31091	40	not required
Zentiva Pharm…	Panthenol ointment Lichtenst…	EH4594	31764	60	not required

Validation samples

A total of 70 089 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 *Panthenol ointment Lichtenstein*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Panthenol ointment Lichtenstein*.

- 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
Zentiva Pharma GmbH	Panthenol ointment Lichtenst…	GC5567	33284	40
Zentiva Pharma GmbH	Panthenol ointment Lichtenst…	GD5661	33425	40

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 *Panthenol ointment Lichtenstein*.

- 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.

- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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 *Panthenol ointment Lichtenstein* 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 *Panthenol ointment Lichtenstein* 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	28 415
Type B	0	80	0	26 021
Type C	0	0	0	15 433

The substance/substance group *Panthenol ointment Lichtenstein* 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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Panthenol ointment Lichtenstein* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Stomahesive® adhesive paste	104.50	–

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

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
30727	30727	0.00	190.41
31091	31091	0.00	187.51
31764	31764	0.00	158.60

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Patchouli oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	31547-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	2

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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 *Patchouli 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	Patchouli oil	00475B27	34389	40
Taoasis	Patchouli oil	1633-126207	33031	40
Taoasis	Patchouli oil	P29-1186	34113	40

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Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Patchouli oil	1633-126207	33032	40

- 25 941 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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

- 15 431 spectra from 1165 *Apo-Ident* customers from a total of 5022 batches from a further 158 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	28 355
Type B	0	72	88	25 941
Type C	0	2	0	15 431

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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9509 %)	45.0000 % (> 43.1250 %)
Type C	100.0000 % (> 98.9905 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Patchouli oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	16.41	–
Lemon grass oil	23.66	–
Tea tree oil	29.61	–
Carrot seed oil	29.81	–
Cedar wood oil	34.12	–
Dwarf pine oil	36.37	–
Immortelle oil	43.85	–
Melissa oil	47.94	–
Cypress oil	49.80	–
Citronella oil	49.89	–

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.

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	23.66
31619	31619	0.00	35.97
32172	32172	0.00	36.80
37669	37669	0.00	41.51

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Peppermint oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30930-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	142

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 355 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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.

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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

- 25 861 spectra from a total of 582 batches from further 209 substances. These spectra were recorded by *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.

- 278 spectra from 204 *Apo-Ident* customers from 144 batches from the substance/substance group *Peppermint oil*.

- Among them are spectra of independent samples from 140 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	22000613006	1
Alliance	Peppermint oil	22000130024	2
Apotheke Bauer & Cie. o...	Peppermint oil		1
bambastus	Peppermint oil	21002270	1
Bombaltus	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	1
Bombastus	Peppermint oil	286204	1
Bombastus	Peppermint oil	303064	1
Bombastus	Peppermint oil	307854	3
Caelo	Peppermint oil	12114225	1
Caelo	Peppermint oil	1319I-01995	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

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Supplier	Substance	Batch	Spectra
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	5
Caelo	Peppermint oil	18221725	1
Caelo	Peppermint oil	19000776001	1
Caelo	Peppermint oil	19000776010	1
Caelo	Peppermint oil	191136001	1
Caelo	Peppermint oil	19113601	1
Caelo	Peppermint oil	19113603	1
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	6
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	18
Caelo	Peppermint oil	20003483002	1
Caelo	Peppermint oil	20003483006	8
Caelo	Peppermint oil	20003483009	1
Caelo	Peppermint oil	20003483011	1
Caelo	Peppermint oil	20003483014	5
Caelo	Peppermint oil	20003483015	1
Caelo	Peppermint oil	20003589001	2
Caelo	Peppermint oil	2000358901	1
Caelo	Peppermint oil	20003795002	2
Caelo	Peppermint oil	20003795005	2
Caelo	Peppermint oil	20003795010	1
Caelo	Peppermint oil	20003991003	3
Caelo	Peppermint oil	2000648008	1
Caelo	Peppermint oil	2003483014	1
Caelo	Peppermint oil	22000130001	1
Caelo	Peppermint oil	22000130003	3
Caelo	Peppermint oil	22000130008	1
Caelo	Peppermint oil	22000130020	1
Caelo	Peppermint oil	22000613006	1
Caelo	Peppermint oil	617Q-01995	1
Caelo	Peppermint oil	9135901	1
Caelo	Peppermint oil	W474	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Ph...	Peppermint oil	20003795010	1
Caesar & Loretz GmbH	Peppermint oil	20000648008	3
Caesar & Loretz GmbH	Peppermint oil	20003483014	3
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	20003483006	1
Euro OTC	Peppermint oil	1231489	1
Euro OTC	Peppermint oil	16114611	1
Euro OTC	Peppermint oil	1804008-01	1
Euro OTC	Peppermint oil	180400802	1
Euro OTC	Peppermint oil	1804008-02	3
Euro OTC	Peppermint oil	19005885	1
Euro OTC	Peppermint oil	2011012-01	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	1
Fagron	Peppermint oil	20C16-B07-201867	3
Fagron	Peppermint oil	21/17-T08-090070	1
Fagron	Peppermint oil	21117-T06-093899	1
Fagron	Peppermint oil	21E12-086267	1
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
Hänseler	Peppermint oil		1
Kögl	Peppermint oil	421211154615	1
Melsan	Peppermint oil	1705811	1
Noweda	Peppermint oil	1900776010	1
Noweda	Peppermint oil	20000648008	1
Noweda	Peppermint oil	22002982001	1
Ph/Euro	Peppermint oil	170303202	1
Phoenix 28.12..18	Peppermint oil	18221702	1
Phoenix	Peppermint oil	19135905	1
Phönix	Peppermint oil	22000376	1
Primavera	Peppermint oil	191K27	1
Primavera	Peppermint oil	291C29	1
Primavera	Peppermint oil	61M27	1
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
Taoasis	Peppermint oil	111455-6397	3
Taoasis	Peppermint oil	123108-7608	1
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

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Supplier	Substance	Batch	Spectra
Taoasis	Peppermint oil	65074-125102BAG90451	1
Taoasis	Peppermint oil	75404-127882	1
Taoasis	Peppermint oil	78725-128653	1
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
Toasis/Noweda	Peppermint oil		2

- 15 155 spectra from 1152 *Apo-Ident* customers from a total of 4882 batches from a further 158 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	28 355
Type B	0	222	18	25 861
Type C	0	262	16	15 155

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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9509 %)	92.5000 % (> 91.2500 %)
Type C	100.0000 % (> 98.9650 %)	94.2446 % (> 93.1655 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Peppermint oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

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Substance	Distance in main model	Distance in second-stage model
Marjoram oil	61.19	–

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.

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	86.31
30965	30965	0.00	94.72
32481	32481	0.00	71.57
33809	33809	0.00	68.58
37785	37785	0.00	70.20

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 2.5-2023-04

Validated substance/substance group	**Perfume oil vanilla**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30665-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Perfume oil vanilla; Oleum vanillae planifoliae

Special notes

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

- Advice: Currently no longer available. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Perfume oil vanilla	3	1	2

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Perfume oil vanilla*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Perfume oil vanilla	10293212	30665	40	not required
Caelo	Perfume oil vanilla	13393501	31191	40	1403100
Caelo	Perfume oil vanilla	13393501	31400	40	not required
Caelo	Perfume oil vanilla	14284107	31786	60	not required

Validation samples

A total of 70 089 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 *Perfume oil vanilla*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 375 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Perfume oil vanilla*.
- 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
Caelo	Perfume oil vanilla	15316308	33439	40
Caelo	Perfume oil vanilla	15316308	33440	40

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- 26 021 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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 7 *Apo-Ident* customers from 2 batches from the substance/substance group *Perfume oil vanilla*.

- 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	Perfume oil vanilla	15316308	12
Caelo	Perfume oil vanilla	17054404	2
Caesar & Loretz GmbH	Perfume oil vanilla	17054404	1

- 15 418 spectra from 1165 *Apo-Ident* customers from a total of 5022 batches from a further 158 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 *Perfume oil vanilla* 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 *Perfume oil vanilla* 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	28 375
Type B	0	80	0	26 021
Type C	0	15	0	15 418

The substance/substance group *Perfume oil vanilla* 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 % (> 99.9638 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9682 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Perfume oil vanilla* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Salmon oil	84.32	–

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

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
30665	30665	0.00	124.63
31191	31191	0.00	121.24
31400	31400	0.00	122.02
31786	31786	0.00	131.43

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Raspberry aroma**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30562-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	4	102

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 355 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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 *Raspberry 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.

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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

- 25 941 spectra from a total of 584 batches from further 209 substances. These spectra were recorded by *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.

- 450 spectra from 235 *Apo-Ident* customers from 107 batches from the substance/substance group *Raspberry aroma*.
- Among them are spectra of independent samples from 102 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
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	5
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	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

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Supplier	Substance	Batch	Spectra
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	14
Caelo	Raspberry aroma	180743307	1
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	5
Caelo	Raspberry aroma	19160002	21
Caelo	Raspberry aroma	19160006	8
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	12
Caelo	Raspberry aroma	192776007	1
Caelo	Raspberry aroma	192776008	1
Caelo	Raspberry aroma	192776009	1
Caelo	Raspberry aroma	192776010	4
Caelo	Raspberry aroma	20002006001	1
Caelo	Raspberry aroma	20002006002	1
Caelo	Raspberry aroma	20002006003	15
Caelo	Raspberry aroma	20002006006	4
Caelo	Raspberry aroma	210000063011	1
Caelo	Raspberry aroma	21000063004	10
Caelo	Raspberry aroma	21000063005	1
Caelo	Raspberry aroma	21000063008	5
Caelo	Raspberry aroma	2100063011	1
Caelo	Raspberry aroma	21002109001	1
Caelo	Raspberry aroma	21002129001	5
Caelo	Raspberry aroma	21002129002	2
Caelo	Raspberry aroma	21002129006	5
Caelo	Raspberry aroma	21002129009	2
Caelo	Raspberry aroma	21002129011	1
Caelo	Raspberry aroma	2100219006	1
Caelo	Raspberry aroma	2100219010	1
Caelo	Raspberry aroma	2102129006	1
Caelo	Raspberry aroma	210512-05	1
Caelo	Raspberry aroma	217258101	1
Caelo	Raspberry aroma	22000122002	4
Caelo	Raspberry aroma	22000122006	6
Caelo	Raspberry aroma	22000122008	1
Caelo	Raspberry aroma	22000122010	1
Caelo	Raspberry aroma	22000122011	5
Caelo	Raspberry aroma	22000122013	1
Caelo	Raspberry aroma	22002419002	1

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Supplier	Substance	Batch	Spectra
Caelo	Raspberry aroma	22002419003	2
Caelo	Raspberry aroma	22003420001	3
Caelo	Raspberry aroma	22003420010	2
Caelo	Raspberry aroma	22003420016	1
Caelo	Raspberry aroma	220808(22000122006)	1
Caeolo	Raspberry aroma	14376103	1
Caesar & Lorenz	Raspberry aroma	22003420001	1
Caesar & Loretz GmbH / ...	Raspberry aroma	192776006	1
Caesar & Loretz GmbH / ...	Raspberry aroma	18249907	1
Caesar & Loretz GmbH /G...	Raspberry aroma	192776006	1
Caesar & Loretz GmbH/ AHD	Raspberry aroma	19160002	1
Caesar & Loretz GmbH/ G...	Raspberry aroma	20002006006	1
Caesar & Loretz GmbH/ G...	Raspberry aroma	18249902	1
Caesar & Loretz GmbH/No...	Raspberry aroma	19160001	1
Caesar & Loretz GmbH/Ph...	Raspberry aroma	22000122011	1
Caesar & Loretz GmbH/sana	Raspberry aroma	192776001	1
Caesar & Loretz GmbH/Sa...	Raspberry aroma	19160001	1
Caesar & Loretz GmbH/Sa...	Raspberry aroma	192776010	1
Caesar & Loretz GmbH/Sa...	Raspberry aroma	20002006003	1
Caesar & Loretz GmbH/Sa...	Raspberry aroma	21000063008	1
Caesar & Loretz GmbH/Sa...	Raspberry aroma	22000122012	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	1
Caesar & Loretz GmbH	Raspberry aroma	19160008	1
Caesar & Loretz GmbH	Raspberry aroma	192776001	1
Caesar & Loretz GmbH	Raspberry aroma	192776006	5
Caesar & Loretz GmbH	Raspberry aroma	192776010	1
Caesar & Loretz GmbH	Raspberry aroma	20002006002	1
Caesar & Loretz GmbH	Raspberry aroma	20002006003	7
Caesar & Loretz GmbH	Raspberry aroma	20002006006	1
Caesar & Loretz GmbH	Raspberry aroma	21000063004	2
Caesar & Loretz GmbH	Raspberry aroma	21000063008	8
Caesar & Loretz GmbH	Raspberry aroma	21002129001	1
Caesar & Loretz GmbH	Raspberry aroma	21002129006	1
Caesar & Loretz GmbH	Raspberry aroma	21002129009	1
Caesar & Loretz GmbH	Raspberry aroma	22000122002	2
Caesar & Loretz GmbH	Raspberry aroma	22000122005	1
Caesar & Loretz GmbH	Raspberry aroma	22000122006	3
Caesar & Loretz GmbH	Raspberry aroma	22000122011	1
Caesar & Loretz GmbH	Raspberry aroma	22002419003	1
Caesar & Loretz GmbH	Raspberry aroma	22002419006	1
Caesar & Loretz GmbH	Raspberry aroma	22003420005	1
Caesar & Loretz Hilden/...	Raspberry aroma	19160006	1
Caesar & Loretz Hilden	Raspberry aroma	19160002	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

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Supplier	Substance	Batch	Spectra
Gehe	Raspberry aroma	21002129009	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
Noveda	Raspberry aroma	210000063008	1
Noweda/ Caesar&Lorenz G…	Raspberry aroma	192776001	1
Noweda	Raspberry aroma	14115909	1
Noweda	Raspberry aroma	17258101	1
Noweda	Raspberry aroma	18249905	1
Noweda	Raspberry aroma	20002006003	1
Phoenix	Raspberry aroma	17258106	1
Phoenix	Raspberry aroma	18249910	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
Rondell Apotheke	Raspberry aroma	15438501	1
Sanacorp	Raspberry aroma	19160002	1
Sanacorp	Raspberry aroma	22000122002	1
Sanacorp	Raspberry aroma	22003420016	1

- 14 983 spectra from 1142 *Apo-Ident* customers from a total of 4917 batches from a further 158 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	28 355
Type B	0	160	0	25 941
Type C	0	448	2	14 983

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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 98.9649 %)	99.5556 % (> 98.8889 %)

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.)

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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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Raspberry aroma* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Strawberry aroma	36.08	–
Contramarum aroma	53.16	–

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.

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	66.61
31396	31396	0.00	70.65
33222	33222	0.00	75.16
36049	36737	5.72	53.65
36737	36737	0.00	57.32

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 2.5-2023-04

Validated substance/substance group	**Ravensara oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30386-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ravensara oil; Ravensara (essentiel oil)

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Ravensara oil	2	3	14

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Ravensara oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Ravensara oil	231012-118739	31635	60	not required
Taoasis	Ravensara oil	1687-966	33854	40	not required
Taoasis	Ravensara oil	1687-966	33872	40	not required

Validation samples

A total of 70 089 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 *Ravensara oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 28 415 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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 *Ravensara 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	Ravensara oil	00065B27	34403	40
Taoasis	Ravensara oil	1687-125316	32803	40
Taoasis	Ravensara oil	1994-3103	34285	40
Taoasis	Ravensara oil	1687-125316	33029	40

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- 25 941 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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 1 *Apo-Ident* customers from 15 batches from the substance/substance group *Ravensara oil*.

- Among them are spectra of independent samples from 14 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	Ravensara oil	1687-125316	1
Taoasis	Ravensara oil	1687-126824	1
Taoasis	Ravensara oil	1687-127661	1
Taoasis	Ravensara oil	1944-1388	1
Taoasis	Ravensara oil	1944-1733	1
Taoasis	Ravensara oil	1994-3103	1
Taoasis	Ravensara oil	2101005-116830	3
Taoasis	Ravensara oil	231012-118738	1
Taoasis	Ravensara oil	231012-118739	2
Taoasis	Ravensara oil	231012-118892	1
Taoasis	Ravensara oil	231012-119831	1
Taoasis	Ravensara oil	231012-120291	1
Taoasis	Ravensara oil	2427-5280	1
Taoasis	Ravensara oil	59/144/17	1
Taoasis	Ravensara oil	9331006-121650	3

- 15 413 spectra from 1165 *Apo-Ident* customers from a total of 5009 batches from a further 158 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 *Ravensara 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 *Ravensara 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	140	0	28 415
Type B	0	160	0	25 941
Type C	0	20	0	15 413

The substance/substance group *Ravensara 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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 98.9674 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Ravensara oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Hyssop oil	13.17	–
Sage oil	17.23	–
Rosemary oil	23.42	–
Citus oil	28.91	–
Marjoram oil	29.00	–
Angelica root oil	35.01	–
Rosemary camphor oil	37.26	–
Cypress oil	40.41	–
Yarrow oil	41.21	–
Eucalyptus oil	42.17	–
Myrtle oil	42.36	–
Niaouli oil	46.59	–
Cajeput (essentiel oil)	48.11	–

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

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	23.01
33854	33854	0.00	23.77
33872	33872	0.00	24.05

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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 2.5-2023-04

Validated substance/substance group	**Rose oil, pure**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`34034-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	1	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

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 475 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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 *Rose oil, pure*.
- 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	Rose oil, pure	00099L26	34405	40

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- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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.
- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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	28 475
Type B	0	0	40	26 061
Type C	0	0	0	15 433

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 % (> 99.9642 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9514 %)	0.0000 % (≥ 0.0000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Rose oil, pure* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Palmarosa oil, organic	52.64	–

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.

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	59.70
37790	37790	0.00	99.79

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Rose-geranium oil, organic**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30536-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	2	31

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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 4 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 3 different batches.

- 28 335 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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.

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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

- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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.

- 37 spectra from 13 *Apo-Ident* customers from 31 batches from the substance/substance group *Rose-geranium oil, organic*.

- 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
apomix	Rose-geranium oil, organic	2260-2431	1
Biofrid	Rose-geranium oil, organic	5010	1
Bombastus	Rose-geranium oil, organic	22625-106677	1
Primavera/Primavera	Rose-geranium oil, organic	618L23	1
primavera	Rose-geranium oil, organic	177G27	1
Primavera	Rose-geranium oil, organic	8304131	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
Taoasis	Rose-geranium oil, organic	130111-110467	1
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

- 15 396 spectra from 1165 *Apo-Ident* customers from a total of 4993 batches from a further 158

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	220	0	28 335
Type B	0	120	0	25 981
Type C	0	37	0	15 396

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 % (> 99.9637 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9662 %)	100.0000 % (> 83.7838 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Rose-geranium oil, organic* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Citronella oil	24.57	–
alpha-bisabolol (racemic) at least 85%	34.41	–
Marjoram oil	49.55	–
Carrot seed oil	52.48	–

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.

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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	32.96
31776	31776	0.00	33.90
31951	31951	0.00	33.59
33036	33036	0.00	27.18

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 2.5-2023-04

Validated substance/substance group	**Rosemary camphor oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	33803-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	1

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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*

Validation samples

A total of 70 089 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.
- 28 405 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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.

*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
Primavera	Rosemary camphor oil	00179G26	34170	40
Primavera	Rosemary camphor oil	00631A27	34373	40

- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Rosemary camphor 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	Rosemary camphor oil	794L27	1

- 15 432 spectra from 1165 *Apo-Ident* customers from a total of 5023 batches from a further 158 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	28 405
Type B	0	80	0	26 021
Type C	0	1	0	15 432

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 % (> 99.9638 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.0163 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Rosemary camphor oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Rosemary oil	10.97	–
Hyssop oil	17.10	–
Citus oil	17.10	–
Eucalyptus oil	21.66	–
Ravensara oil	25.55	–
Niaouli oil	30.44	–
Cajeput (essentiel oil)	34.04	–
Myrtle oil	35.46	–
Marjoram oil	36.19	–
Spruce needle oil	36.44	–
Sage oil	36.90	–
Cypress oil	42.28	–
Angelica root oil	46.57	–

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.

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	20.44
33959	33959	0.00	20.06
35733	35733	0.00	16.84
35734	35734	0.00	19.19

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

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variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Rosewood oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31556-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Rosewood oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 395 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 25 981 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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/Taoasis	Rosewood oil	109177-5863	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
Taoasis	Rosewood oil	5101015-124967	3
Taoasis	Rosewood oil	5101017-122566	2
Taoasis	Rosewood oil	9177-3983	2

- 15 402 spectra from 1165 *Apo-Ident* customers from a total of 5008 batches from a further 158 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	160	0	28 395
Type B	0	120	0	25 958
Type C	0	31	0	15 402

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 % (> 99.9638 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9513 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9665 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Rosewood oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, white	45.89	–
Coriander oil	69.89	–

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.

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	48.22
31688	31688	0.00	54.24
34106	34106	0.00	41.63

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Sage oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31139-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	14

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 375 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 021 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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 8 *Apo-Ident* customers from 14 batches from the substance/substance group *Sage oil*.

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

Supplier	Substance	Batch	Spectra
Bombastus	Sage oil	18004276	2
Bombastus	Sage oil	20004247	2
Bombastus	Sage oil	309857	1
Taoasis/ Phoenix (28.08...	Sage oil	7156ITL06	1
Taoasis/Phoenix/22.03.2...	Sage oil	7156ITL06	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

- 15 413 spectra from 1165 *Apo-Ident* customers from a total of 5011 batches from a further 158 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	28 375
Type B	0	80	0	26 021
Type C	0	18	2	15 413

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 % (> 99.9638 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9674 %)	90.0000 % (> 75.0000 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Sage oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Rosemary camphor oil	18.63	–
Hyssop oil	22.98	–
Spruce needle oil	23.27	–
Rosemary oil	28.90	–
Eucalyptus oil	32.45	–
Matricaria oil, roman	35.25	–
Ravensara oil	38.96	–
Silver fir oil	46.89	–
Marjoram oil	49.23	–

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.

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	36.49
31257	31257	0.00	32.26
31783	31783	0.00	23.27
37672	37672	0.00	38.96

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

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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 2.5-2023-04

Validated substance/substance group	**Salicylic white paraffin 10%**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31521-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Salicylic white paraffin 10%

Special notes

When selecting the *Salicylic white paraffin 10%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Salicylic white paraffin 10%	3	3	17

Second-stage model

For differentiation of the substance/substance group *Salicylic white paraffin 10%* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Salicylic white paraffin 10%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Bombastus	Salicylic white paraffin 10%	287820	31521	60	not required
Bombastus	Salicylic white paraffin 10%	291886	31629	75	not required
Bombastus	Salicylic white paraffin 10%	310227	33473	40	not required

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 175 spectra of 3 reference samples from the substance/substance group *Salicylic white paraffin 10%*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 380 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Salicylic white paraffin 10%*.
- 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	Salicylic white paraffin 10%	302737	32741	40
Bombastus	Salicylic white paraffin 10%	309004	33416	40
Bombastus	Salicylic white paraffin 10%	22004053	36889	40

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- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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.

- 19 spectra from 14 *Apo-Ident* customers from 17 batches from the substance/substance group *Salicylic white paraffin 10%*.

- 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
Bombastus	Salicylic white paraffin 10%	17000464	1
Bombastus	Salicylic white paraffin 10%	19003777	1
Bombastus	Salicylic white paraffin 10%	19004850	1
Bombastus	Salicylic white paraffin 10%	293212	1
Caelo	Salicylic white paraffin 10%	15394702	1
Caelo	Salicylic white paraffin 10%	16120701	2
Caelo	Salicylic white paraffin 10%	16214202	1
Caelo	Salicylic white paraffin 10%	16214203	1
Caelo	Salicylic white paraffin 10%	18114703	1
Caelo	Salicylic white paraffin 10%	18245603	1
Caelo	Salicylic white paraffin 10%	19058602	1
Caelo	Salicylic white paraffin 10%	19140601	2
Caelo	Salicylic white paraffin 10%	21000468001	1
Eigenrezeptur	Salicylic white paraffin 10%	150702	1
Medicon Apotheke Defektur	Salicylic white paraffin 10%	4818J-07017	1
Winthrop Arzneimittel	Salicylic white paraffin 10%	IE6931	1
Winthrop	Salicylic white paraffin 10%	GA0926	1

- 15 414 spectra from 1164 *Apo-Ident* customers from a total of 5007 batches from a further 158 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 *Salicylic white paraffin 10%* 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 *Salicylic white paraffin 10%* 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	175	0	28 380
Type B	0	120	0	25 981
Type C	0	19	0	15 414

The substance/substance group *Salicylic white paraffin 10%* 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 % (> 99.9638 %)	100.0000 % (> 96.5714 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9675 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Salicylic white paraffin 10%* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Cottonwood ointment	41.80	–
Wax ointment (stabilised)	48.04	–
Neribas® fat ointment	48.68	–
Marjoram ointment	54.74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Salicylic white paraffin 10%* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

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
31521	31521	0.00	61.52
31629	31629	0.00	61.21
33473	33473	0.00	61.02

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,

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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 2.5-2023-04

Validated substance/substance group	**Salmon oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	33088-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Salmon oil

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Salmon oil	3	3	1

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Salmon oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Salmon oil	170345	33088	40	20170213*
Caelo	Salmon oil	173079	34225	40	20171116*
Caelo	Salmon oil	21004006	36160	40	20211216*

Validation samples

A total of 70 089 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 *Salmon oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 435 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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.

- 130 spectra of 3 reference samples from the substance/substance group *Salmon 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.

*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	Salmon oil	182524	34341	40
Caelo	Salmon oil	20000795	35034	40
Caelo	Salmon oil	21003192	35788	50

- 25 971 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Salmon 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
Sanacorp	Salmon oil	20003591001	1

- 15 432 spectra from 1165 *Apo-Ident* customers from a total of 5023 batches from a further 158 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 *Salmon 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 *Salmon 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	28 435
Type B	0	130	0	25 971
Type C	0	1	0	15 432

The substance/substance group *Salmon 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 % (> 99.9639 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.0163 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Salmon oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Balm Bio Nature	47.68	–
Argan oil	49.40	–
Cedar wood oil	73.40	–

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

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
33088	33088	0.00	47.68
34225	34225	0.00	54.71
36160	36160	0.00	56.13

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Sandalwood oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	33799-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Sandalwood oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 435 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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

- 15 429 spectra from 1165 *Apo-Ident* customers from a total of 5022 batches from a further 158 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	120	0	28 435
Type B	0	120	0	25 981
Type C	0	4	0	15 429

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 % (> 99.9639 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9777 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Sandalwood oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Rose oil, pure	95.91	–

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.

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	104.29
33801	33801	0.00	109.77
33832	33832	0.00	95.91

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Savory herb**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	33820-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	2	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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Savory herb*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 28 475 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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

- 15 429 spectra from 1165 *Apo-Ident* customers from a total of 5021 batches from a further 158 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	80	0	28 475
Type B	0	40	0	26 061
Type C	0	4	0	15 429

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 % (> 99.9642 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9514 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.9777 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Savory herb* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Thyme oil, red	22.97	–
Oregano oil	39.69	–

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.

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	25.70
33821	33821	0.00	22.97

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Sebexol® / Wofacutan / Hans Karrer**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30839-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sebexol® / Wofacutan / Hans Karrer; Hans Karrer Hydrocream MicroSilver; Sebexol® basic pH 5 formula basis; Sebexol® cream lotion pH 5; Wofacutan wash lotion

Special notes

When selecting the *Sebexol® / Wofacutan / Hans Karrer* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	17	9	216

Second-stage model

For differentiation of the substance/substance group *Sebexol®* / *Wofacutan* / *Hans Karrer* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Hans Karrer G…	Hans Karrer Hydrocream Micro…	16001	33190	40	not required
Hans Karrer G…	Hans Karrer Hydrocream Micro…	16002	33191	40	not required
Hans Karrer G…	Hans Karrer Hydrocream Micro…	18002	34116	40	not required
Hans Karrer G…	Hans Karrer Hydrocream Micro…	22004	36726	40	not required
Hans Karrer G…	Hans Karrer Hydrocream Micro…	22002	36727	40	not required
Devesa	Sebexol® basic pH 5 formula …	1307	31104	40	1403098
Devesa	Sebexol® basic pH 5 formula …	1522	31961	60	not required
Devesa	Sebexol® basic pH 5 formula …	1638124	32744	40	not required
Devesa	Sebexol® cream lotion pH 5	1220	30839	40	1403097
Devesa	Sebexol® cream lotion pH 5	1317	31103	40	not required
Devesa	Sebexol® cream lotion pH 5	1412	31592	45	not required
Devesa	Sebexol® cream lotion pH 5	1531	31839	60	not required
Devesa	Sebexol® cream lotion pH 5	1552.2	32743	40	not required
Devesa	Sebexol® cream lotion pH 5	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 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 765 spectra of 17 reference samples from the substance/substance group *Sebexol®* / *Wofacutan* / *Hans Karrer*. These samples are listed above in the *calibration samples* section. The reference samples come from 17 different batches.
- 27 790 spectra from a total of 588 batches from further 156 substances. These spectra were recorded by *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 by *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:

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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.

- 450 spectra of 11 reference samples from the substance/substance group *Sebexol®* / *Wofacutan* / *Hans Karrer*.
- 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
Hans Karrer GmbH	Hans Karrer Hydrocream Micro…	16003	33192	40
Hans Karrer GmbH	Hans Karrer Hydrocream Micro…	16004	33193	40
Hans Karrer GmbH	Hans Karrer Hydrocream Micro…	21003	35574	50
Devesa	Sebexol® basic pH 5 formula …	1712122	33427	40
Devesa	Sebexol® basic pH 5 formula …	1644102	33432	40
Devesa	Sebexol® basic pH 5 formula …	2243126	37424	40
Devesa	Sebexol® cream lotion pH 5	1605101	32907	40
Kesla Pharma	Wofacutan wash lotion	0729.16	32913	40
Kesla Pharma	Wofacutan wash lotion	0061.22	36772	40
Devesa	Sebexol® cream lotion pH 5	1605101	32908	40
Kesla Pharma	Wofacutan wash lotion	0729.16	32914	40

- 25 651 spectra from a total of 579 batches from further 206 substances. These spectra were recorded by *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.

- 1439 spectra from 211 *Apo-Ident* customers from 213 batches from the substance/substance group *Sebexol®* / *Wofacutan* / *Hans Karrer*.
- Among them are spectra of independent samples from 182 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® cream lotion pH 5	2149110	1
2128114/AHD	Sebexol® cream lotion pH 5	2128114	1
Astellas	Sebexol® cream lotion pH 5	1504	2
Bombastus	Sebexol® basic pH 5 formula …	1346	2
Caelo	Sebexol® cream lotion pH 5		2
Caelo	Sebexol® basic pH 5 formula …	1131	2
Caelo	Sebexol® basic pH 5 formula …	1239	1
Caelo	Sebexol® cream lotion pH 5	1417	1
Caelo	Sebexol® cream lotion pH 5	1430	1
Caelo	Sebexol® basic pH 5 formula …	1440	1
Caelo	Sebexol® cream lotion pH 5	1504	1
Caelo	Sebexol® cream lotion pH 5	1511	2
Caelo	Sebexol® cream lotion pH 5	1531	1
Caelo	Sebexol® basic pH 5 formula …	1604127	2
Caelo	Sebexol® cream lotion pH 5	1604129	1
Caelo	Sebexol® cream lotion pH 5	1605101	3

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Supplier	Substance	Batch	Spectra
Caelo	Sebexol® basic pH 5 formula ...	1620117	2
Caelo	Sebexol® cream lotion pH 5	1708120	3
Caelo	Sebexol® cream lotion pH 5	1712223	1
Caelo	Sebexol® cream lotion pH 5	1719112	1
Caelo	Sebexol® cream lotion pH 5	1727207	1
Caelo	Sebexol® cream lotion pH 5	1736105	3
Caelo	Sebexol® basic pH 5 formula ...	1746116	2
Caelo	Sebexol® cream lotion pH 5	1802208	1
Caelo	Sebexol® cream lotion pH 5	1807113	2
Caelo	Sebexol® cream lotion pH 5	1812123	2
Caelo	Sebexol® basic pH 5 formula ...	1817126	1
Caelo	Sebexol® cream lotion pH 5	1817227	1
Caelo	Sebexol® cream lotion pH 5	1824215	1
Caelo	Sebexol® cream lotion pH 5	1828110	1
Caelo	Sebexol® cream lotion pH 5	1836106	1
Caelo	Sebexol® basic pH 5 formula ...	1851119	2
Caelo	Sebexol® cream lotion pH 5	19031605	1
Caelo	Sebexol® cream lotion pH 5	1912119	1
Caelo	Sebexol® cream lotion pH 5	1912120	1
Caelo	Sebexol® cream lotion pH 5	4117E-03872	1
Chiesi GmbH	Sebexol® basic pH 5 formula ...	1851119	1
Chiesi	Sebexol® cream lotion pH 5	218112	1
Deversa/Fiebig	Sebexol® cream lotion pH 5	1817127	1
Deversa/Fiebig	Sebexol® cream lotion pH 5	1824115	1
Deversa/Noweda	Sebexol® basic pH 5 formula ...	1644102	1
Deversa/Noweda	Sebexol® basic pH 5 formula ...	1712122	1
Deversa/Noweda	Sebexol® basic pH 5 formula ...	1719111	1
Deversa/Noweda	Sebexol® basic pH 5 formula ...	1807113	1
Deversa/Noweda	Sebexol® basic pH 5 formula ...	1817126	1
Deversa/Noweda	Sebexol® basic pH 5 formula ...	1923107	1
Deversa/Noweda	Sebexol® basic pH 5 formula ...	2031128	1
deversa	Sebexol® cream lotion pH 5	1935227	5
Deves/Phönix	Sebexol® cream lotion pH 5	2127109	1
Devesa Fiebig	Sebexol® cream lotion pH 5	2128112	1
Devesa / AHD	Sebexol® cream lotion pH 5	1939227	1
Devesa / AHD	Sebexol® cream lotion pH 5	1947118	1
Devesa / AHD	Sebexol® cream lotion pH 5	2009227	2
DEVESA / Anzag	Sebexol® cream lotion pH 5	1605101	1
DEVESA / Anzag	Sebexol® cream lotion pH 5	1802208	1
Devesa / Dr. Reingraber...	Sebexol® basic pH 5 formula ...	2009126	1
Devesa / Dr. Reingraber...	Sebexol® basic pH 5 formula ...	2031128	1
Devesa / Dr. Reingraber...	Sebexol® basic pH 5 formula ...	2102114	1
devesa / Fiebig	Sebexol® cream lotion pH 5	1736106	1
devesa / Fiebig	Sebexol® cream lotion pH 5	1743125	1
devesa / Fiebig	Sebexol® cream lotion pH 5	1746116	1
devesa / Fiebig	Sebexol® cream lotion pH 5	1802208	1
devesa / Fiebig	Sebexol® cream lotion pH 5	1812123	1
devesa / Fiebig	Sebexol® cream lotion pH 5	1828110	1
devesa / Fiebig	Sebexol® cream lotion pH 5	1912120	1
devesa / Fiebig	Sebexol® cream lotion pH 5	1935227	1
Devesa / Fiebig	Sebexol® cream lotion pH 5	2009127	1
Devesa / G	Sebexol® basic pH 5 formula ...	2009126	1
Devesa / Gehe 08.12.18	Sebexol® cream lotion pH 5	1824215-S20190115Ma7	1
Devesa / Gehe 15.3.18	Sebexol® cream lotion pH 5	1743225-20180404Ma10	1
Devesa / Gehe	Sebexol® cream lotion pH 5		1
Devesa / Gehe	Sebexol® cream lotion pH 5	1517	1
Devesa / Gehe	Sebexol® cream lotion pH 5	1530	2
Devesa / Gehe	Sebexol® cream lotion pH 5	1651120	1
Devesa / Gehe	Sebexol® cream lotion pH 5	1727107	1
Devesa / Gehe	Sebexol® cream lotion pH 5	1736106	2

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Supplier	Substance	Batch	Spectra
Devesa / Gehe	Sebexol® cream lotion pH 5	1746116	3
Devesa / Gehe	Sebexol® basic pH 5 formula ...	1817126	1
Devesa / Gehe	Sebexol® cream lotion pH 5	1824215	2
Devesa / Gehe	Sebexol® basic pH 5 formula ...	1851119	1
Devesa / Gehe	Sebexol® basic pH 5 formula ...	1912118	1
Devesa / Gehe	Sebexol® cream lotion pH 5	1923108	1
Devesa / Gehe	Sebexol® basic pH 5 formula ...	1935126	2
Devesa / Gehe	Sebexol® cream lotion pH 5	1935127	1
Devesa / Gehe	Sebexol® basic pH 5 formula ...	2009126	3
Devesa / Gehe	Sebexol® cream lotion pH 5	2009127	1
Devesa / Gehe	Sebexol® cream lotion pH 5	2019107	2
Devesa / Gehe	Sebexol® cream lotion pH 5	2045106	1
Devesa / Kehr	Sebexol® basic pH 5 formula ...	1644102	1
Devesa / Noweda	Sebexol® cream lotion pH 5	1430	1
Devesa / Noweda	Sebexol® cream lotion pH 5	1531	1
Devesa / Noweda	Sebexol® basic pH 5 formula ...	1620117	1
Devesa / Noweda	Sebexol® basic pH 5 formula ...	1638124	1
Devesa / Noweda	Sebexol® cream lotion pH 5	1644102	1
Devesa / Noweda	Sebexol® basic pH 5 formula ...	170420S/1620117	1
Devesa / Noweda	Sebexol® basic pH 5 formula ...	170516S/1644102	1
DEVESA / Noweda	Sebexol® basic pH 5 formula ...	1712122	3
Devesa / Noweda	Sebexol® cream lotion pH 5	1712223	1
Devesa / Noweda	Sebexol® cream lotion pH 5	1720115	1
Devesa / Noweda	Sebexol® cream lotion pH 5	1736106	2
Devesa / Noweda	Sebexol® cream lotion pH 5	1802208	1
Devesa / Noweda	Sebexol® cream lotion pH 5	1807113	1
Devesa / Noweda	Sebexol® cream lotion pH 5	1836105	3
Devesa / Noweda	Sebexol® cream lotion pH 5	1912119	1
Devesa / Noweda	Sebexol® cream lotion pH 5	2019207	3
Devesa / Noweda	Sebexol® cream lotion pH 5	2045106	1
Devesa / Phönix	Sebexol® cream lotion pH 5	1812123	1
Devesa / Phönix	Sebexol® cream lotion pH 5	2004120	1
Devesa / Phönix	Sebexol® cream lotion pH 5	2009127	1
Devesa / Sanacorp	Sebexol® cream lotion pH 5	1828111	2
Devesa /	Sebexol® cream lotion pH 5	1511	1
Devesa /	Sebexol® cream lotion pH 5	1812223	1
Devesa /	Sebexol® cream lotion pH 5	1912119	1
Devesa /	Sebexol® cream lotion pH 5	1923108	2
DEVESA /G	Sebexol® basic pH 5 formula ...	1912118	1
Devesa /Gehe	Sebexol® cream lotion pH 5	1901103	1
DEVESA /K	Sebexol® basic pH 5 formula ...	1946114	1
Devesa /Noweda	Sebexol® cream lotion pH 5	1901103	2
Devesa /Phönix	Sebexol® cream lotion pH 5	1807113	9
Devesa /phönix	Sebexol® cream lotion pH 5	1947118	1
Devesa Dr. Reingraber G...	Sebexol® basic pH 5 formula ...	1828110	1
Devesa Dr. Reingraber G...	Sebexol® basic pH 5 formula ...	1923107	2
DEVESA Dr. Reingraber G...	Sebexol® cream lotion pH 5	21281147	1
Devesa Dr. Reingraber G...	Sebexol® basic pH 5 formula ...	2124115	1
Devesa Dr. Reingraber G...	Sebexol® cream lotion pH 5	2124116	1
Devesa Dr. Reingraber G...	Sebexol® cream lotion pH 5	2127208	3
DEVESA Dr. Reingraber G...	Sebexol® cream lotion pH 5	2149108	1
Devesa DR. Reingraber	Sebexol® cream lotion pH 5	1651121	1
Devesa Dr.Reingraben/Sa...	Sebexol® cream lotion pH 5	1743125	1
Devesa Dr.Reingraben/Sa...	Sebexol® cream lotion pH 5	1817127	3
DEVESA Dr.Reingraber Gm...	Sebexol® cream lotion pH 5	2127109	1
DEVESA Dr.Reingraber Gm...	Sebexol® cream lotion pH 5	2128112	5
DEVESA Dr.Reingraber Gm...	Sebexol® cream lotion pH 5	2128114	1
Devesa Dr.Reingraber Gm...	Sebexol® basic pH 5 formula ...	1244	1
Devesa Dr.Reingraber Gm...	Sebexol® basic pH 5 formula ...	1303	1
Devesa Dr.Reingraber Gm...	Sebexol® basic pH 5 formula ...	1935126	1

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Supplier	Substance	Batch	Spectra
Devesa Dr.Reingraber Gm...	Sebexol® basic pH 5 formula ...	2031128	1
DEVESA Dr.Reingraber GmbH	Sebexol® basic pH 5 formula ...	1328	1
Devesa Dr.Reingraber GmbH	Sebexol® basic pH 5 formula ...	1425	1
Devesa Dr.Reingraber GmbH	Sebexol® basic pH 5 formula ...	1644102	2
Devesa Dr.Reingraber GmbH	Sebexol® cream lotion pH 5	174611650ml	1
Devesa Dr.Reingraber GmbH	Sebexol® cream lotion pH 5	1935127	1
Devesa Dr.Reingraber GmbH	Sebexol® cream lotion pH 5	2009227	1
Devesa Dr.Reingraber GmbH	Sebexol® basic pH 5 formula ...	2045106	1
Devesa Dr.Reingraber/Sa...	Sebexol® cream lotion pH 5	1925121	1
Devesa Dr.Reingraber/Sa...	Sebexol® cream lotion pH 5	1939127	3
Devesa GmbH /Alliance H...	Sebexol® cream lotion pH 5	1712223	1
Devesa GmbH /Alliance H...	Sebexol® cream lotion pH 5	1828110	1
Devesa GmbH /Alliance H...	Sebexol® cream lotion pH 5	1828111	1
devesa Noweda	Sebexol® cream lotion pH 5	1802208	1
devesa phoenix	Sebexol® cream lotion pH 5	1925121	1
devesa phoenix	Sebexol® cream lotion pH 5	1947119	1
devesa phoenix	Sebexol® cream lotion pH 5	2009227	2
Devesa- Phönix	Sebexol® basic pH 5 formula ...	1604127	1
Devesa, Geibo	Sebexol® cream lotion pH 5	2128114	1
Devesa/ Noweda	Sebexol® basic pH 5 formula ...	1712122	1
Devesa/ Noweda	Sebexol® cream lotion pH 5	1817227	1
Devesa/ AHD	Sebexol® cream lotion pH 5	2019107	1
Devesa/ AHD	Sebexol® cream lotion pH 5	2127108	3
Devesa/ Ebert	Sebexol® basic pH 5 formula ...	1817126	1
Devesa/ Fiebig	Sebexol® basic pH 5 formula ...	1338	1
Devesa/ Fiebig	Sebexol® cream lotion pH 5	1447	1
Devesa/ Fiebig	Sebexol® cream lotion pH 5	1712223	2
Devesa/ Fiebig	Sebexol® cream lotion pH 5	1935227	1
Devesa/ Noweda	Sebexol® cream lotion pH 5	1736105	1
Devesa/ Noweda	Sebexol® cream lotion pH 5	1802208	1
Devesa/ Noweda	Sebexol® cream lotion pH 5	1807113	1
Devesa/ Noweda	Sebexol® cream lotion pH 5	1901103	1
Devesa/ Noweda	Sebexol® cream lotion pH 5	1935227	2
Devesa/ Noweda	Sebexol® cream lotion pH 5	1939227	4
Devesa/ Noweda	Sebexol® cream lotion pH 5	1947118	1
Devesa/ Noweda	Sebexol® cream lotion pH 5	1947119	2
DEVESA/ Noweda	Sebexol® basic pH 5 formula ...	2124115	1
Devesa/ Noweda	Sebexol® cream lotion pH 5	2124116	1
Devesa/ Phoenix	Sebexol® basic pH 5 formula ...	1543	1
Devesa/ Phoenix	Sebexol® cream lotion pH 5	1620117	1
Devesa/ Phoenix	Sebexol® cream lotion pH 5	1817127	1
DEVESA/ Phoenix	Sebexol® cream lotion pH 5	1939127/09	1
Devesa/ Phoenix	Sebexol® basic pH 5 formula ...	2127106	5
Devesa/ Phönix	Sebexol® cream lotion pH 5	1524	1
Devesa/ Phönix	Sebexol® cream lotion pH 5	1727207	1
Devesa/ Phönix	Sebexol® cream lotion pH 5	1736105	2
Devesa/ Phönix	Sebexol® cream lotion pH 5	1736106	6
Devesa/ Phönix	Sebexol® cream lotion pH 5	1743225	2
Devesa/ Phönix	Sebexol® cream lotion pH 5	1812223	3
DEVESA/ Phönix	Sebexol® cream lotion pH 5	2040130	1
Devesa/ Sanacorp	Sebexol® cream lotion pH 5	1912120	1
Devesa/ Sanacorp	Sebexol® cream lotion pH 5	1923108	1
Devesa/ Sanacorp	Sebexol® cream lotion pH 5	1925121	1
Devesa/ Sanacorp	Sebexol® cream lotion pH 5	1939127	1
Devesa/ Sanacorp	Sebexol® cream lotion pH 5	20042120	1
Devesa/	Sebexol® cream lotion pH 5		2
Devesa/	Sebexol® cream lotion pH 5	1504	2
Devesa/	Sebexol® cream lotion pH 5	1524	1
Devesa/	Sebexol® cream lotion pH 5	1604129	4
Devesa/	Sebexol® cream lotion pH 5	1644102	1

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Supplier	Substance	Batch	Spectra
Devesa/	Sebexol® cream lotion pH 5	17433225	1
Devesa/	Sebexol® cream lotion pH 5	1947118	1
Devesa/AHD	Sebexol® basic pH 5 formula ...	1245	4
Devesa/AHD	Sebexol® basic pH 5 formula ...	1328	7
Devesa/AHD	Sebexol® cream lotion pH 5	1912119	1
Devesa/AHD	Sebexol® cream lotion pH 5	1947118	1
Devesa/AHD	Sebexol® cream lotion pH 5	2009127	2
Devesa/AHD	Sebexol® cream lotion pH 5	2040130	1
Devesa/AHD	Sebexol® cream lotion pH 5	2045106	1
Devesa/AHD	Sebexol® cream lotion pH 5	2103119	1
Devesa/AHD	Sebexol® cream lotion pH 5	2103120	1
Devesa/AHD	Sebexol® cream lotion pH 5	2128114	1
Devesa/Alliance	Sebexol® basic pH 5 formula ...	1644102	1
Devesa/Alliance	Sebexol® cream lotion pH 5	1923108	2
Devesa/Alliance	Sebexol® cream lotion pH 5	1935127	2
Devesa/Alliance	Sebexol® cream lotion pH 5	1939227	1
Devesa/Alliance	Sebexol® basic pH 5 formula ...	1946114	2
Devesa/Alliance	Sebexol® basic pH 5 formula ...	2009126	5
Devesa/Alliance	Sebexol® cream lotion pH 5	2019207	1
Devesa/Alliance	Sebexol® basic pH 5 formula ...	2031128	16
Devesa/Alliance	Sebexol® cream lotion pH 5	2046109	2
Devesa/Alliance	Sebexol® basic pH 5 formula ...	2149108	6
Devesa/Alliance	Sebexol® basic pH 5 formula ...	2243126	1
Devesa/Anzag	Sebexol® cream lotion pH 5		2
Devesa/Anzag	Sebexol® cream lotion pH 5	2004120	1
DEVESA/Anzag	Sebexol® cream lotion pH 5	2127208	1
Devesa/fiebig	Sebexol® cream lotion pH 5		1
Devesa/Fiebig	Sebexol® cream lotion pH 5		1
Devesa/Fiebig	Sebexol® cream lotion pH 5	1426	1
Devesa/Fiebig	Sebexol® cream lotion pH 5	1511	1
Devesa/Fiebig	Sebexol® cream lotion pH 5	1712123	2
Devesa/Fiebig	Sebexol® cream lotion pH 5	1736105	5
Devesa/Fiebig	Sebexol® cream lotion pH 5	1824115	2
DEVESA/Fiebig	Sebexol® cream lotion pH 5	1925121	1
Devesa/Fiebig	Sebexol® cream lotion pH 5	1935127	2
DEVESA/Fiebig	Sebexol® cream lotion pH 5	1935127	1
DEVESA/Fiebig	Sebexol® cream lotion pH 5	1939227	1
Devesa/Fiebig	Sebexol® cream lotion pH 5	1947118	6
DEVESA/Fiebig	Sebexol® cream lotion pH 5	1947118	1
Devesa/Fiebig	Sebexol® cream lotion pH 5	1947119	2
DEVESA/Fiebig	Sebexol® cream lotion pH 5	1947119	1
Devesa/Fiebig	Sebexol® cream lotion pH 5	2004120	1
Devesa/Fiebig	Sebexol® cream lotion pH 5	2009127	4
Devesa/Fiebig	Sebexol® cream lotion pH 5	201107	2
Devesa/Fiebig	Sebexol® cream lotion pH 5	2019107	6
Devesa/Fiebig	Sebexol® cream lotion pH 5	2019207	1
Devesa/Fiebig	Sebexol® cream lotion pH 5	2040130	2
Devesa/Fiebig	Sebexol® cream lotion pH 5	2045106	3
Devesa/Fiebig	Sebexol® cream lotion pH 5	2046109	1
Devesa/Fiebig	Sebexol® cream lotion pH 5	2103119	4
Devesa/Fiebig	Sebexol® cream lotion pH 5	2103120	2
Devesa/Fiebig	Sebexol® cream lotion pH 5	2124116	2
Devesa/Fiebig	Sebexol® cream lotion pH 5	2124117	1
Devesa/Gehe	Sebexol® basic pH 5 formula ...		1
devesa/gehe	Sebexol® basic pH 5 formula ...	1346	1
devesa/gehe	Sebexol® basic pH 5 formula ...	1356	1
Devesa/Gehe	Sebexol® cream lotion pH 5	1504	1
Devesa/Gehe	Sebexol® cream lotion pH 5	1644102	1
Devesa/Gehe	Sebexol® cream lotion pH 5	1651121	1
Devesa/Gehe	Sebexol® cream lotion pH 5	1712123	1

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Supplier	Substance	Batch	Spectra
Devesa/Gehe	Sebexol® cream lotion pH 5	1817227	1
Devesa/Gehe	Sebexol® cream lotion pH 5	1828111	1
Devesa/Gehe	Sebexol® cream lotion pH 5	1836106	1
Devesa/Gehe	Sebexol® basic pH 5 formula ...	1851119	1
Devesa/Gehe	Sebexol® basic pH 5 formula ...	1912118	1
Devesa/Gehe	Sebexol® cream lotion pH 5	1912119	1
Devesa/Gehe	Sebexol® basic pH 5 formula ...	1923107	2
Devesa/Gehe	Sebexol® basic pH 5 formula ...	1935126	2
Devesa/Gehe	Sebexol® cream lotion pH 5	1939127	1
Devesa/Gehe	Sebexol® basic pH 5 formula ...	1946114	1
Devesa/Gehe	Sebexol® cream lotion pH 5	2009227	2
Devesa/Gehe	Sebexol® cream lotion pH 5	2127108	2
DEVESA/Gehe	Sebexol® cream lotion pH 5	2127208	1
Devesa/Gehe	Sebexol® cream lotion pH 5	2128114	1
Devesa/Jenne	Sebexol® cream lotion pH 5	2103119	2
Devesa/Kehr/25.05.2020	Sebexol® cream lotion pH 5	2004120	2
Devesa/Kehr	Sebexol® basic pH 5 formula ...	1407	2
Devesa/Kehr	Sebexol® basic pH 5 formula ...	1620117	1
Devesa/Kehr	Sebexol® basic pH 5 formula ...	1923107	1
Devesa/Kehr	Sebexol® basic pH 5 formula ...	1946114	1
Devesa/Kehr	Sebexol® basic pH 5 formula ...	1946114/11	1
Devesa/Kehr	Sebexol® basic pH 5 formula ...	2009126	3
Devesa/Kehr	Sebexol® basic pH 5 formula ...	2102114	2
Devesa/Kehr	Sebexol® basic pH 5 formula ...	2124115	1
Devesa/Krieger	Sebexol® cream lotion pH 5	1802108	1
Devesa/Krieger	Sebexol® cream lotion pH 5	1901102	1
Devesa/Krieger	Sebexol® cream lotion pH 5	1901103	1
Devesa/Krieger	Sebexol® cream lotion pH 5	1939227	1
Devesa/Krieger	Sebexol® cream lotion pH 5	1947118	1
Devesa/Krieger	Sebexol® cream lotion pH 5	2004120	2
Devesa/Noveda	Sebexol® cream lotion pH 5	2124166	1
Devesa/NOW	Sebexol® cream lotion pH 5		1
Devesa/NOW	Sebexol® cream lotion pH 5	1504	2
Devesa/NOW	Sebexol® cream lotion pH 5	1504/01	1
Devesa/NOW	Sebexol® cream lotion pH 5	1523	1
Devesa/NOW	Sebexol® cream lotion pH 5	1552	1
Devesa/NOW	Sebexol® cream lotion pH 5	1604129	1
Devesa/NOW	Sebexol® cream lotion pH 5	1604228	1
Devesa/NOW	Sebexol® cream lotion pH 5	1644102	1
Devesa/NOW	Sebexol® cream lotion pH 5	1901103	1
Devesa/NOW	Sebexol® cream lotion pH 5	2019207	1
Devesa/Noweda	Sebexol® cream lotion pH 5		3
Devesa/Noweda	Sebexol® basic pH 5 formula ...	1430	1
Devesa/Noweda	Sebexol® basic pH 5 formula ...	1440	2
Devesa/Noweda	Sebexol® cream lotion pH 5	1447	3
Devesa/Noweda	Sebexol® cream lotion pH 5	1543	1
DEVESA/Noweda	Sebexol® basic pH 5 formula ...	1543	1
Devesa/Noweda	Sebexol® basic pH 5 formula ...	1604127	1
DEVESA/Noweda	Sebexol® basic pH 5 formula ...	1604127	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1604228	6
Devesa/Noweda	Sebexol® cream lotion pH 5	1604328	5
Devesa/Noweda	Sebexol® cream lotion pH 5	1605103	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1605201	3
DEVESA/Noweda	Sebexol® cream lotion pH 5	1605201	2
Devesa/Noweda	Sebexol® basic pH 5 formula ...	1638124	2
Devesa/Noweda	Sebexol® cream lotion pH 5	1651120	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1651121	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1708120	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1712123	1
Devesa/Noweda	Sebexol® basic pH 5 formula ...	1719111/05	1

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Devesa/Noweda	Sebexol® cream lotion pH 5	1719112	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1720115	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1736105	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1736106	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1743225	1
Devesa/Noweda	Sebexol® basic pH 5 formula ...	1807113	2
Devesa/Noweda	Sebexol® cream lotion pH 5	1812223	1
Devesa/Noweda	Sebexol® basic pH 5 formula ...	1817126	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1817227	3
Devesa/Noweda	Sebexol® cream lotion pH 5	1824115	1
Devesa/Noweda	Sebexol® basic pH 5 formula ...	1828110	2
Devesa/Noweda	Sebexol® basic pH 5 formula ...	1828110/07	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1828111	2
Devesa/Noweda	Sebexol® cream lotion pH 5	1901102	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1912119	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1923108	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1935127	2
Devesa/Noweda	Sebexol® cream lotion pH 5	1935227	1
Devesa/Noweda	Sebexol® cream lotion pH 5	1939127	2
Devesa/Noweda	Sebexol® cream lotion pH 5	1939227	4
Devesa/Noweda	Sebexol® basic pH 5 formula ...	1946114	3
Devesa/Noweda	Sebexol® cream lotion pH 5	1947118	2
Devesa/Noweda	Sebexol® cream lotion pH 5	1947119	10
Devesa/Noweda	Sebexol® cream lotion pH 5	1947119/11	1
Devesa/Noweda	Sebexol® cream lotion pH 5	2004120	4
Devesa/Noweda	Sebexol® cream lotion pH 5	200412D	1
Devesa/Noweda	Sebexol® basic pH 5 formula ...	2009126	1
Devesa/Noweda	Sebexol® cream lotion pH 5	2009227	3
Devesa/Noweda	Sebexol® cream lotion pH 5	2040130	4
Devesa/Noweda	Sebexol® cream lotion pH 5	2045106	1
Devesa/Noweda	Sebexol® cream lotion pH 5	2103119	1
DEVESA/Noweda	Sebexol® cream lotion pH 5	2124116	1
Devesa/Noweda	Sebexol® cream lotion pH 5	2127108	2
DEVESA/Noweda	Sebexol® cream lotion pH 5	2127108	5
Devesa/Noweda	Sebexol® cream lotion pH 5	2127208	2
Devesa/Noweda	Sebexol® cream lotion pH 5	2128112	3
Devesa/Noweda	Sebexol® cream lotion pH 5	2128114	1
Devesa/Noweda	Sebexol® cream lotion pH 5	2149110	2
DEVESA/Phoenix	Sebexol® basic pH 5 formula ...	1446/11	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	1511	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	1746116	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	1807113	3
Devesa/Phoenix	Sebexol® cream lotion pH 5	1824215	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	1828111	2
Devesa/Phoenix	Sebexol® cream lotion pH 5	1901102	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	1901103	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	1912120	3
Devesa/Phoenix	Sebexol® cream lotion pH 5	1925121	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	1939127	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	1947118	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	1947119	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	2004120	1
Devesa/Phoenix	Sebexol® cream lotion pH 5	2009227	3
Devesa/Phoenix	Sebexol® cream lotion pH 5	2045106	1
Devesa/Phoenix	Sebexol® basic pH 5 formula ...	2102114	17
Devesa/Phoenix	Sebexol® basic pH 5 formula ...	2124115	12
Devesa/Phoenix	Sebexol® cream lotion pH 5	2124117	2
Devesa/Phoenix	Sebexol® basic pH 5 formula ...	2304125	1
Devesa/Phömix	Sebexol® cream lotion pH 5	1712223	2
Devesa/Phönix	Sebexol® basic pH 5 formula ...	1543	3

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Supplier	Substance	Batch	Spectra
Devesa/Phönix	Sebexol® basic pH 5 formula ...	1620117	2
Devesa/Phönix	Sebexol® basic pH 5 formula ...	1638124	2
Devesa/Phönix	Sebexol® cream lotion pH 5	1708120	1
Devesa/Phönix	Sebexol® basic pH 5 formula ...	1712122	2
DEVESA/Phönix	Sebexol® basic pH 5 formula ...	1719111	1
devesa/Phönix	Sebexol® cream lotion pH 5	1727107	1
Devesa/Phönix	Sebexol® cream lotion pH 5	1727207	1
devesa/Phönix	Sebexol® cream lotion pH 5	1743125	5
devesa/Phönix	Sebexol® cream lotion pH 5	1746116	8
Devesa/Phönix	Sebexol® cream lotion pH 5	1746116	1
devesa/Phönix	Sebexol® cream lotion pH 5	1802208	5
Devesa/Phönix	Sebexol® cream lotion pH 5	1807113	2
DEVESA/Phönix	Sebexol® basic pH 5 formula ...	1807113	1
Devesa/Phönix	Sebexol® cream lotion pH 5	1807113/02	1
Devesa/Phönix	Sebexol® cream lotion pH 5	1817227	1
devesa/Phönix	Sebexol® cream lotion pH 5	18201402	1
Devesa/Phönix	Sebexol® cream lotion pH 5	1824115	2
devesa/Phönix	Sebexol® cream lotion pH 5	1824215	2
Devesa/Phönix	Sebexol® cream lotion pH 5	1824215	1
DEVESA/Phönix	Sebexol® basic pH 5 formula ...	1828110	1
Devesa/Phönix	Sebexol® cream lotion pH 5	1828111	19
Devesa/Phönix	Sebexol® cream lotion pH 5	1836105	2
DEVESA/Phönix	Sebexol® basic pH 5 formula ...	1851119	1
DEVESA/Phönix	Sebexol® cream lotion pH 5	185119	1
Devesa/Phönix	Sebexol® cream lotion pH 5	1901102	2
Devesa/Phönix	Sebexol® cream lotion pH 5	1901103	6
Devesa/Phönix	Sebexol® cream lotion pH 5	19107	1
Devesa/Phönix	Sebexol® cream lotion pH 5	1912119	1
Devesa/Phönix	Sebexol® cream lotion pH 5	1912120	3
Devesa/Phönix	Sebexol® cream lotion pH 5	1923108	9
Devesa/Phönix	Sebexol® cream lotion pH 5	1925121	1
Devesa/Phönix	Sebexol® cream lotion pH 5	1935127	1
Devesa/Phönix	Sebexol® cream lotion pH 5	1935227	6
Devesa/Phönix	Sebexol® cream lotion pH 5	1939127	7
DEVESA/Phönix	Sebexol® cream lotion pH 5	1947119	2
Devesa/Phönix	Sebexol® cream lotion pH 5	2004120	2
Devesa/Phönix	Sebexol® cream lotion pH 5	2009227	8
Devesa/Phönix	Sebexol® cream lotion pH 5	2019107	1
Devesa/Phönix	Sebexol® basic pH 5 formula ...	2031128	2
Devesa/Phönix	Sebexol® cream lotion pH 5	2045106	1
Devesa/Phönix	Sebexol® cream lotion pH 5	2124116	2
DEVESA/Phönix	Sebexol® cream lotion pH 5	2124117	1
Devesa/Phönix	Sebexol® cream lotion pH 5	2127208	1
Devesa/Sanacorp WE: 09....	Sebexol® cream lotion pH 5	1651121	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1440	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1511	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1522	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1530	2
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1543	4
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1620117	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1638124	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1644102	2
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1712122	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1719111	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1743125	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1746116	2
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1802108	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1807113	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1817126	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1817127	1

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Supplier	Substance	Batch	Spectra
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1828110	3
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1828111	4
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1836105	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1836106	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1851119	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	187126/06	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1901102	2
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1912120	2
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1923107	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1925121	2
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	1935126	4
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1935127	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1935227	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1939227	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1947118	2
Devesa/Sanacorp	Sebexol® cream lotion pH 5	1947119	1
DEVESA/Sanacorp	Sebexol® cream lotion pH 5	2004120	2
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	2009126	2
Devesa/Sanacorp	Sebexol® cream lotion pH 5	2019207	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	2031128	5
Devesa/Sanacorp	Sebexol® cream lotion pH 5	2040130	3
Devesa/Sanacorp	Sebexol® cream lotion pH 5	2103119	1
Devesa/Sanacorp	Sebexol® basic pH 5 formula ...	2124115	5
Devesa/Sanacorp	Sebexol® cream lotion pH 5	2124117	1
Devesa/Sanacorp	Sebexol® cream lotion pH 5	2127108	1
Devesa	Sebexol® basic pH 5 formula ...		9
Devesa	Sebexol® basic pH 5 formula ...	1232	1
Devesa	Sebexol® basic pH 5 formula ...	1239	1
Devesa	Sebexol® basic pH 5 formula ...	1307	5
DEVESA	Sebexol® basic pH 5 formula ...	1318	2
Devesa	Sebexol® basic pH 5 formula ...	1328	5
DEVESA	Sebexol® basic pH 5 formula ...	1328	2
Devesa	Sebexol® basic pH 5 formula ...	1335	2
Devesa	Sebexol® basic pH 5 formula ...	1404	1
Devesa	Sebexol® basic pH 5 formula ...	1407	2
Devesa	Sebexol® cream lotion pH 5	1417N-03872	1
Devesa	Sebexol® basic pH 5 formula ...	1430	1
Devesa	Sebexol® basic pH 5 formula ...	1440	4
DEVESA	Sebexol® basic pH 5 formula ...	1440	2
DEVESA	Sebexol® cream lotion pH 5	1505	1
Devesa	Sebexol® cream lotion pH 5	1510	4
DEVESA	Sebexol® cream lotion pH 5	1510	1
Devesa	Sebexol® basic pH 5 formula ...	1511	2
DEVESA	Sebexol® basic pH 5 formula ...	1511	1
Devesa	Sebexol® basic pH 5 formula ...	1522	3
Devesa	Sebexol® cream lotion pH 5	1523	3
DEVESA	Sebexol® cream lotion pH 5	1523	1
Devesa	Sebexol® cream lotion pH 5	1524	1
DEVESA	Sebexol® cream lotion pH 5	1531	1
Devesa	Sebexol® basic pH 5 formula ...	1543	6
Devesa	Sebexol® basic pH 5 formula ...	1604127	4
Devesa	Sebexol® cream lotion pH 5	1604128	1
Devesa	Sebexol® cream lotion pH 5	1604129	1
Devesa	Sebexol® cream lotion pH 5	1604328	1
Devesa	Sebexol® cream lotion pH 5	1605103	1
Devesa	Sebexol® basic pH 5 formula ...	1620117	2
Devesa	Sebexol® basic pH 5 formula ...	1638124	3
Devesa	Sebexol® basic pH 5 formula ...	1644102	5
DEVESA	Sebexol® basic pH 5 formula ...	1644102	1
DEVESA	Sebexol® cream lotion pH 5	1651120	2

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Supplier	Substance	Batch	Spectra
Devesa	Sebexol® cream lotion pH 5	1651121	3
Devesa	Sebexol® basic pH 5 formula ...	1683124	1
Devesa	Sebexol® cream lotion pH 5	1708120	4
DEVESA	Sebexol® cream lotion pH 5	1708120	1
Devesa	Sebexol® basic pH 5 formula ...	1712122	4
DEVESA	Sebexol® basic pH 5 formula ...	1712122	1
devesa	Sebexol® basic pH 5 formula ...	1719111	3
Devesa	Sebexol® basic pH 5 formula ...	1719111	3
DEVESA	Sebexol® basic pH 5 formula ...	1719111	1
Devesa	Sebexol® cream lotion pH 5	1727107	2
Devesa	Sebexol® cream lotion pH 5	1736105	1
DEVESA	Sebexol® cream lotion pH 5	1736105	1
Devesa	Sebexol® cream lotion pH 5	1736106	1
Devesa	Sebexol® cream lotion pH 5	1743125	1
Devesa	Sebexol® cream lotion pH 5	1743225	1
DEVESA	Sebexol® cream lotion pH 5	1743225	1
devesa	Sebexol® cream lotion pH 5	1746116	1
Devesa	Sebexol® basic pH 5 formula ...	1746116	5
Devesa	Sebexol® cream lotion pH 5	1802108/01	1
DEVESA	Sebexol® cream lotion pH 5	1802108/01	1
Devesa	Sebexol® cream lotion pH 5	1802208	1
Devesa	Sebexol® basic pH 5 formula ...	1807113	2
DEVESA	Sebexol® basic pH 5 formula ...	1807113	3
DEVESA	Sebexol® cream lotion pH 5	1812123	2
Devesa	Sebexol® cream lotion pH 5	1812223	7
Devesa	Sebexol® basic pH 5 formula ...	1817126	1
DEVESA	Sebexol® basic pH 5 formula ...	1817126	1
Devesa	Sebexol® cream lotion pH 5	1817127	3
Devesa	Sebexol® cream lotion pH 5	1817227	2
DEVESA	Sebexol® cream lotion pH 5	1817227	1
Devesa	Sebexol® cream lotion pH 5	1824115	5
DEVESA	Sebexol® cream lotion pH 5	1824215	1
Devesa	Sebexol® basic pH 5 formula ...	1828110	4
Devesa	Sebexol® cream lotion pH 5	1828111	1
Devesa	Sebexol® cream lotion pH 5	1836105	1
DEVESA	Sebexol® cream lotion pH 5	1836106	2
Devesa	Sebexol® basic pH 5 formula ...	1851119	4
DEVESA	Sebexol® basic pH 5 formula ...	185119	1
Devesa	Sebexol® cream lotion pH 5	1901102	6
Devesa	Sebexol® cream lotion pH 5	1901103	5
DEVESA	Sebexol® cream lotion pH 5	1901103	1
Devesa	Sebexol® basic pH 5 formula ...	1912118	4
DEVESA	Sebexol® basic pH 5 formula ...	1912118	1
Devesa	Sebexol® cream lotion pH 5	1912119	3
Devesa	Sebexol® cream lotion pH 5	1912120	2
DEVESA	Sebexol® cream lotion pH 5	1912120	1
Devesa	Sebexol® basic pH 5 formula ...	1923107	6
DEVESA	Sebexol® basic pH 5 formula ...	1923107	1
Devesa	Sebexol® cream lotion pH 5	1923108	3
Devesa	Sebexol® cream lotion pH 5	1923108/06-2022	1
Devesa	Sebexol® cream lotion pH 5	1925120	1
Devesa	Sebexol® cream lotion pH 5	1925121	8
DEVESA	Sebexol® cream lotion pH 5	1925121	1
Devesa	Sebexol® basic pH 5 formula ...	1935126	2
DEVESA	Sebexol® basic pH 5 formula ...	1935126	1
Devesa	Sebexol® cream lotion pH 5	1935127	3
Devesa	Sebexol® cream lotion pH 5	1935227	5
Devesa	Sebexol® cream lotion pH 5	1939127	1
Devesa	Sebexol® cream lotion pH 5	1939227	2
DEVESA	Sebexol® cream lotion pH 5	1939227	2

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Devesa	Sebexol® basic pH 5 formula ...	1946114	6
Devesa	Sebexol® cream lotion pH 5	1947118	3
Devesa	Sebexol® cream lotion pH 5	1947119	5
Devesa	Sebexol® cream lotion pH 5	2004120	4
Devesa	Sebexol® basic pH 5 formula ...	2009126	4
DEVESA	Sebexol® basic pH 5 formula ...	2009126	1
Devesa	Sebexol® cream lotion pH 5	2009127	2
Devesa	Sebexol® cream lotion pH 5	2009227	4
Devesa	Sebexol® cream lotion pH 5	201907	1
Devesa	Sebexol® cream lotion pH 5	2019107	4
Devesa	Sebexol® cream lotion pH 5	2019207	7
Devesa	Sebexol® basic pH 5 formula ...	2031128	3
DEVESA	Sebexol® basic pH 5 formula ...	2031128	1
Devesa	Sebexol® cream lotion pH 5	2040130	6
Devesa	Sebexol® cream lotion pH 5	2045106	9
Devesa	Sebexol® cream lotion pH 5	2046109	3
DEVESA	Sebexol® cream lotion pH 5	2046109	1
Devesa	Sebexol® basic pH 5 formula ...	2102114	1
DEVESA	Sebexol® basic pH 5 formula ...	2102114	1
Devesa	Sebexol® cream lotion pH 5	2103119	5
Devesa	Sebexol® cream lotion pH 5	2103120	8
Devesa	Sebexol® basic pH 5 formula ...	2124115	1
Devesa	Sebexol® cream lotion pH 5	2124116	4
Devesa	Sebexol® cream lotion pH 5	2124117	7
Devesa	Sebexol® cream lotion pH 5	2127108	4
Devesa	Sebexol® cream lotion pH 5	2127109	2
Devesa	Sebexol® cream lotion pH 5	2127208	1
Devesa	Sebexol® cream lotion pH 5	2128114	1
Devesa	Sebexol® cream lotion pH 5	2149110	1
Devesa	Sebexol® cream lotion pH 5	250322/1	1
Devesa	Sebexol® cream lotion pH 5	9072021	1
Devesa	Sebexol® basic pH 5 formula ...	I232	1
Devesa	Sebexol® basic pH 5 formula ...	I307	1
Devesa-Fa.Gehe	Sebexol® cream lotion pH 5	1727207/-20180112Ma9	1
Devesa-Fa.Gehe	Sebexol® cream lotion pH 5	1824215-S20181115Ma2	1
DevesaSanacorp	Sebexol® cream lotion pH 5	1912119	1
Devesea	Sebexol® cream lotion pH 5	1604128	1
Dewesa/Kehr	Sebexol® basic pH 5 formula ...	1817126	1
Dewesa/Kehr	Sebexol® basic pH 5 formula ...	1923107	1
Divesa	Sebexol® cream lotion pH 5	1812223	1
Dr Reinhard GmbH- Kehr	Sebexol® basic pH 5 formula ...	1620117	1
Dr. Reingraber GmbH / F...	Sebexol® cream lotion pH 5	1824115	1
Dr. Reingraber GmbH/Pho...	Sebexol® basic pH 5 formula ...	2031128	1
Dr. Reingraber GmbH/Phö...	Sebexol® cream lotion pH 5	2103119	2
Dr. Reingraber GmbH	Sebexol® cream lotion pH 5	1605103	1
Dr. Reingraber GmbH	Sebexol® basic pH 5 formula ...	1708120	1
Dr. Reingraber Gmbh	Sebexol® cream lotion pH 5	1817227	1
Dr. Reingraber GmbH	Sebexol® cream lotion pH 5	1923108	1
Dr. Reingraber Gmbh	Sebexol® cream lotion pH 5	1939127	1
Dr. Reingraber GmbH	Sebexol® cream lotion pH 5	2103119	2
Dr. Reingraber GmbH	Sebexol® cream lotion pH 5	2127108	1
Dr. Wolff	Sebexol® cream lotion pH 5		1
Dr.Reingraber GmbH	Sebexol® basic pH 5 formula ...	1232	1
Dr.Reingraber/sanacorp	Sebexol® basic pH 5 formula ...	1719111	1
Dr.Reingraber/sanacorp	Sebexol® basic pH 5 formula ...	1923107	1
Eigenherstellung	Sebexol® basic pH 5 formula ...	1328	1
Euro OTC	Sebexol® cream lotion pH 5	1727207	1
Fa. Devesa/Gehe	Sebexol® cream lotion pH 5	2009227	1
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	1912120	1
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	1935227	2

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Supplier	Substance	Batch	Spectra
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	1947118	1
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	1947119	1
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	2004120	5
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	2009127	1
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	2040130	1
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	2045106	1
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	2046109	2
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	2103120	3
Fa. Devesa/Noweda	Sebexol® cream lotion pH 5	2127208	3
Fa.Devesa/Gehe	Sebexol® cream lotion pH 5	2019107	1
Fa.Devesa/Noweda	Sebexol® cream lotion pH 5	2124117	1
Fagron	Sebexol® basic pH 5 formula ...	1425	1
Fagron	Sebexol® basic pH 5 formula ...	1510	2
Fagron	Sebexol® cream lotion pH 5	1517	1
Fiebig / Devesa	Sebexol® cream lotion pH 5	2019107	1
Fiebig/Devesa	Sebexol® cream lotion pH 5	1817227	1
Fiebig/Devesa	Sebexol® cream lotion pH 5	1836105	2
Fiebig/Devesa	Sebexol® cream lotion pH 5	1912120	1
Fiebig/Devesa	Sebexol® cream lotion pH 5	2009127	1
Fiebig	Sebexol® basic pH 5 formula ...	1511	2
Fiebig	Sebexol® cream lotion pH 5	1605101	2
Fiebig	Sebexol® cream lotion pH 5	1802108	1
Fiebig	Sebexol® cream lotion pH 5	1812223	1
Fiebig	Sebexol® cream lotion pH 5	1828111	1
Fiebig	Sebexol® cream lotion pH 5	1912119	1
Fiebig	Sebexol® cream lotion pH 5	1912120	1
FIEBIG; HERSTELLER DEVE...	Sebexol® cream lotion pH 5	2004120	1
GEHE / DEVESA	Sebexol® cream lotion pH 5	2009127	1
Gehe/Devesa	Sebexol® cream lotion pH 5		1
Gehe	Sebexol® cream lotion pH 5	1605103	1
Gehe	Sebexol® cream lotion pH 5	1727107	1
Gehe	Sebexol® basic pH 5 formula ...	1935126	2
Gehe	Sebexol® cream lotion pH 5	2009227	1
Geibo/Devesa	Sebexol® cream lotion pH 5	1947118	1
Hans Karrer / Anzag	Hans Karrer Hydrocream Micro...	18002	1
Hans Karrer / Noweda	Hans Karrer Hydrocream Micro...	20007	1
Hans Karrer / Phönix	Hans Karrer Hydrocream Micro...	19003	2
Hans Karrer / Phönix	Hans Karrer Hydrocream Micro...	LOT20001	1
Hans Karrer GmbH / Alli...	Hans Karrer Hydrocream Micro...	18004	2
Hans Karrer GmbH / Sana...	Hans Karrer Hydrocream Micro...	19002	3
Hans Karrer GmbH / Sana...	Hans Karrer Hydrocream Micro...	200002	1
Hans Karrer GmbH / Sana...	Hans Karrer Hydrocream Micro...	20004	1
Hans Karrer GmbH /107	Hans Karrer Hydrocream Micro...	LOT19001	1
Hans Karrer/Alliance	Hans Karrer Hydrocream Micro...	18003	2
Hans Karrer/Phönix	Hans Karrer Hydrocream Micro...	18001	1
hans Karrer/phönix	Hans Karrer Hydrocream Micro...	18003	1
Hans Karrer/Phönix	Hans Karrer Hydrocream Micro...	18003	4
Hans Karrer/Phönix	Hans Karrer Hydrocream Micro...	18004	2
Hans Karrer/Phönix	Hans Karrer Hydrocream Micro...	19001	5
Hans Karrer/Phönix	Hans Karrer Hydrocream Micro...	19003	3
Hans Karrer/Phönix	Hans Karrer Hydrocream Micro...	20001	1
Hans Karrer/Phönix	Hans Karrer Hydrocream Micro...	20005	1
Hans Karrer	Hans Karrer Hydrocream Micro...	21001	2
Hans Karrer	Hans Karrer Hydrocream Micro...	21003	2
Hans Karrer	Hans Karrer Hydrocream Micro...	21005	1
Hans Karrer	Hans Karrer Hydrocream Micro...	LOT20005	1
hanskarrer / Gehe	Hans Karrer Hydrocream Micro...	18001	1
Hanskarrer / Gehe	Hans Karrer Hydrocream Micro...	18002	1
Hanskarrer / Gehe	Hans Karrer Hydrocream Micro...	18003	1
Hanskarrer / Gehe	Hans Karrer Hydrocream Micro...	18004	1

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Supplier	Substance	Batch	Spectra
Hans-Karrer GmbH	Hans Karrer Hydrocream Micro…	18003	1
HansKarrer/Krieger	Hans Karrer Hydrocream Micro…	19003	1
hanskarrer	Hans Karrer Hydrocream Micro…	19004	1
HansKarrerGmbH/Phoekd	Hans Karrer Hydrocream Micro…	20004	1
Hedinger/Noweda	Sebexol® cream lotion pH 5	18424115	1
Holdermann	Sebexol® basic pH 5 formula …	1307	1
Ichthyol Geselschaft Co…	Sebexol® cream lotion pH 5	1836105	1
Ichthyol	Sebexol® basic pH 5 formula …	1232	2
infectopharm/Alliance	Sebexol® cream lotion pH 5	1817227/04	1
Jäger/Noweda	Hans Karrer Hydrocream Micro…	21003	1
Jenne	Hans Karrer Hydrocream Micro…	19001	1
Karrer/Noweda	Hans Karrer Hydrocream Micro…	21003	1
Karrer/Phönix	Hans Karrer Hydrocream Micro…	18004	1
Karrer/Phönix	Hans Karrer Hydrocream Micro…	19001	1
Kehr 14.08.2020	Sebexol® cream lotion pH 5	2009227	1
Kehr/ Devesa	Sebexol® basic pH 5 formula …	1644102	1
Kehr/ Devesa	Sebexol® basic pH 5 formula …	1746116	4
Kehr/Devesa	Sebexol® basic pH 5 formula …	1817126	2
Kehr/Devesa	Sebexol® basic pH 5 formula …	1828110	2
Kesla Pharma/Noweda	Wofacutan wash lotion		2
Kesla Pharma/Phönix	Wofacutan wash lotion	23819	2
Kesla Pharma/Phönix	Wofacutan wash lotion	58118	1
Kesla/Noweda	Wofacutan wash lotion		7
Leo- Pharm	Sebexol® cream lotion pH 5	1828111	1
Max Weber Apotheke	Sebexol® cream lotion pH 5	2009227	1
Noweda / Dewesa	Sebexol® basic pH 5 formula …	1719111	1
NOWEDA / HERSTELLER: DE…	Sebexol® cream lotion pH 5		1
Noweda /Devesa	Sebexol® basic pH 5 formula …	1644102	3
Noweda/Devesa	Sebexol® cream lotion pH 5	1530	1
Noweda/Devesa	Sebexol® cream lotion pH 5	1605201	1
Noweda/Devesa	Sebexol® cream lotion pH 5	1638124	1
Noweda/Devesa	Sebexol® cream lotion pH 5	1720115	1
Noweda/Devesa	Sebexol® cream lotion pH 5	1812123	1
Noweda/devesa	Sebexol® cream lotion pH 5	1836106	1
Noweda/devesa	Sebexol® cream lotion pH 5	1923108	1
Noweda/Devesa	Sebexol® cream lotion pH 5	1923108	1
Noweda/devesa	Sebexol® cream lotion pH 5	1925121	1
Noweda/devesa	Sebexol® cream lotion pH 5	1947118	3
Noweda/Devesa	Sebexol® basic pH 5 formula …	2x1407	1
Noweda	Sebexol® basic pH 5 formula …	1328	1
Noweda	Sebexol® cream lotion pH 5	1651120	1
Noweda	Sebexol® cream lotion pH 5	1708120	1
Noweda	Sebexol® cream lotion pH 5	1712223	1
Noweda	Sebexol® cream lotion pH 5	1802108	1
Noweda	Sebexol® cream lotion pH 5	1817227	1
Noweda	Sebexol® cream lotion pH 5	1828111	1
Noweda	Sebexol® cream lotion pH 5	1836105	2
Noweda	Hans Karrer Hydrocream Micro…	19003	1
Noweda	Sebexol® cream lotion pH 5	1901102	1
Noweda	Sebexol® cream lotion pH 5	1901103	1
Noweda	Sebexol® cream lotion pH 5	1912119	1
Noweda	Sebexol® cream lotion pH 5	1912120	1
Noweda	Sebexol® cream lotion pH 5	1923108	1
Noweda	Sebexol® cream lotion pH 5	1925121	2
Noweda	Sebexol® cream lotion pH 5	1947118	1
Noweda	Sebexol® cream lotion pH 5	1947119	3
Noweda	Sebexol® cream lotion pH 5	2004120	1
noweda	Sebexol® basic pH 5 formula …	2009126	1
Noweda	Sebexol® cream lotion pH 5	2019107	1
Noweda	Sebexol® cream lotion pH 5	2019207	1

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Supplier	Substance	Batch	Spectra
Noweda	Sebexol® basic pH 5 formula ...	2031128	1
Noweda	Sebexol® cream lotion pH 5	2040130	1
Noweda	Sebexol® cream lotion pH 5	2046109	1
Noweda	Hans Karrer Hydrocream Micro...	LOT19001	1
Phoenix/Devesa	Sebexol® basic pH 5 formula ...	1215	1
Phoenix/Devesa	Sebexol® basic pH 5 formula ...	1407	1
Phoenix/Devesa	Sebexol® basic pH 5 formula ...	1604127	1
Phoenix/Devesa	Sebexol® cream lotion pH 5	1736105	1
Phoenix/Devesa	Sebexol® cream lotion pH 5	1812123	1
Phoenix	Sebexol® basic pH 5 formula ...	1440	1
Phönix / Devesa	Sebexol® basic pH 5 formula ...	1644102	1
Phönix / Hans Karrer	Hans Karrer Hydrocream Micro...	20001	2
Phönix Gotha	Wofacutan wash lotion	97913	1
Phönix, Devesa, 29.09.2...	Sebexol® basic pH 5 formula ...	2009126	1
Phönix/ Devesa, 14.12.2...	Sebexol® basic pH 5 formula ...	1935126	3
Phönix/Devesa	Sebexol® cream lotion pH 5	1651121	1
Phönix/Devesa	Sebexol® cream lotion pH 5	1712123	1
Phönix/Devesa	Sebexol® cream lotion pH 5	1712223	2
Phönix/Devesa	Sebexol® cream lotion pH 5	1812123	1
Phönix/Devesa	Sebexol® cream lotion pH 5	1817227	2
Phönix/Devesa	Sebexol® cream lotion pH 5	1824115	3
Phönix/Devesa	Sebexol® cream lotion pH 5	182811	1
Phönix/Devesa	Sebexol® cream lotion pH 5	1836105	1
Phönix/Devesa	Sebexol® cream lotion pH 5	1912120	1
Phönix/DEVESA	Sebexol® cream lotion pH 5	1935127	1
Phönix/Devesa	Sebexol® cream lotion pH 5	1935227	2
Phönix/Devesa	Sebexol® cream lotion pH 5	2019107	1
Phönix/Devesa	Sebexol® cream lotion pH 5	2046109	1
Phönix/Devesa	Sebexol® cream lotion pH 5	2103120	1
Phönix	Sebexol® basic pH 5 formula ...	1313	2
Phönix	Sebexol® basic pH 5 formula ...	1416	1
Phönix	Sebexol® basic pH 5 formula ...	1425	2
Phönix	Sebexol® cream lotion pH 5	1604129	1
Phönix	Sebexol® cream lotion pH 5	160422	1
Phönix	Sebexol® cream lotion pH 5	1828111	2
Phönix	Sebexol® cream lotion pH 5	1912120	1
Phönix	Sebexol® cream lotion pH 5	1935227	1
Phönix	Sebexol® cream lotion pH 5	2004120	2
Phönix	Sebexol® cream lotion pH 5	2009227	1
Phönix	Sebexol® cream lotion pH 5	2128112	2
Phönix	Sebexol® cream lotion pH 5	2128114	2
Phönix	Sebexol® cream lotion pH 5	2149110	2
Phönix	Sebexol® cream lotion pH 5	4217A-03872	1
Römerapo.	Sebexol® cream lotion pH 5	1828110	1
Rondell Apotheke	Sebexol® cream lotion pH 5	1523	1
Sana/Devesa	Sebexol® cream lotion pH 5	1935127	1
Sanacorp / Devesa	Sebexol® cream lotion pH 5	1836106	1
sanacorp, 27.9.16,4,312EUR	Sebexol® cream lotion pH 5	1604328	1
SANACORP/Devasa	Sebexol® cream lotion pH 5	1947119	1
Sanacorp	Sebexol® basic pH 5 formula ...	1313	1
Sanacorp	Sebexol® cream lotion pH 5	2124116	1
Sanacorp	Sebexol® cream lotion pH 5	2127208	1
Sebexol/ Noweda	Sebexol® basic pH 5 formula ...	1403	1
Sebexol/ Noweda	Sebexol® basic pH 5 formula ...	1430	1
Sebexol/AHD	Sebexol® basic pH 5 formula ...	1303	2
Sebexol	Sebexol® basic pH 5 formula ...	1313	1
Sebexol	Sebexol® basic pH 5 formula ...	1333	1
Sebexol	Sebexol® cream lotion pH 5	1604129	1
Sebexol	Sebexol® cream lotion pH 5	1812123	1
Taosis	Sebexol® cream lotion pH 5	1828110	1

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Supplier	Substance	Batch	Spectra
THC Pharma	Sebexol® cream lotion pH 5	1727107	1

- 13 994 spectra from 1157 *Apo-Ident* customers from a total of 4817 batches from a further 155 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* 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* 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	765	0	27 790
Type B	0	450	0	25 651
Type C	0	1439	0	13 994

The substance/substance group *Sebexol® / Wofacutan / Hans Karrer* 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 % (> 99.9635 %)	100.0000 % (> 99.2157 %)
Type B	100.0000 % (> 99.9508 %)	100.0000 % (> 98.6667 %)
Type C	100.0000 % (> 98.9649 %)	100.0000 % (> 99.5830 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Sebexol® / Wofacutan / Hans Karrer* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Excipial® U Hydrolotio	13.06	–
Fenistil® Gel	23.22	–
Dimeticone ointment 10% SR	26.36	–
Amciderm® Base cream	26.39	–
SyrSpend® SF pH4 cherry aroma	35.73	–

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Substanz	Distance in main model	Distance in second-stage model
Abitima® clinic face cream	37.08	–
Base cream Taoasis	38.39	–
Aloe vera gel, 10x concentrated	41.48	–
SyrSpend® SF pH4 aroma free	42.16	–
Retterspitz external	43.01	–
Aloe vera gel, 1:1	44.93	–
Water	46.68	–
Nourivan™ Antiox	51.37	–

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

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
30839	30839	0.00	22.96
30972	30972	0.00	21.48
31065	31065	0.00	22.64
31103	31103	0.00	22.18
31104	31104	0.00	19.64
31592	31592	0.00	21.51
31839	31839	0.00	19.01
31961	31961	0.00	18.33
32743	32743	0.00	22.37
32744	32744	0.00	18.13
33190	33190	0.00	24.25
33191	33191	0.00	22.62
33483	33483	0.00	22.43
34116	34116	0.00	21.11
36726	36726	0.00	24.53
36727	36727	0.00	25.99
36773	36773	0.00	15.02

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Siam benzoin**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31490-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Siam benzoin

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	4	2	0

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Primavera	Siam benzoin	3602151	31490	60	not required
Primavera	Siam benzoin	00051M23	31844	60	not required
Primavera	Siam benzoin	00074M26	34388	40	not required
Primavera	Siam benzoin	00483E31	37781	40	not required

Validation samples

A total of 70 089 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*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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*.
- 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	00218C24	32184	40
Primavera	Siam benzoin	00606B26	34171	40

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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*.

- 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.

- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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* 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* 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	28 355
Type B	0	80	0	26 021
Type C	0	0	0	15 433

The substance/substance group *Siam benzoin* 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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Siam benzoin* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Cinnamon bark oil, Ceylon	113.44	–

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

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	113.44
31844	31844	0.00	215.92
34388	34388	0.00	250.25
37781	37781	0.00	260.62

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Solutio Cordes®**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30996-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Solutio Cordes®

Special notes

When selecting the *Solutio Cordes®* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Solutio Cordes®	3	4	23

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Solutio Cordes*®:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Ichthyol	Solutio Cordes®	12B006	30996	40	not required
Ichthyol	Solutio Cordes®	13B001	31076	40	not required
Ichthyol	Solutio Cordes®	21B0003	35755	50	not required

Validation samples

A total of 70 089 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 *Solutio Cordes*®. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 425 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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.

- 220 spectra of 5 reference samples from the substance/substance group *Solutio Cordes*®.
- 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
Ichthyol	Solutio Cordes®	15B005	32065	60
Ichthyol	Solutio Cordes®	17B007	34361	40
Ichthyol	Solutio Cordes®	19B007	34845	40
Ichthyol	Solutio Cordes®	22B0004	37775	40

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Supplier	Substance	Batch	Sample ID	Spectra
Ichthyol	Solutio Cordes®	15B005	32483	40

- 25 881 spectra from a total of 584 batches from further 209 substances. These spectra were recorded by *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.

- 93 spectra from 40 *Apo-Ident* customers from 27 batches from the substance/substance group *Solutio Cordes®*.

- 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
Cordes/Sanacorp	Solutio Cordes®	19B005	2
Fagron	Solutio Cordes®	17B007	2
Fiebig	Solutio Cordes®	22314	1
Gehe/Ichthyol	Solutio Cordes®	14b006	1
Ichthol/ Noweda 13.11.18	Solutio Cordes®	17b007	1
Ichthyol / E	Solutio Cordes®	15B005	3
Ichthyol / G	Solutio Cordes®	14B012	1
Ichthyol / G	Solutio Cordes®	16B005	3
Ichthyol / Gehe	Solutio Cordes®	14B006	1
Ichthyol /Noweda	Solutio Cordes®	12B005	1
Ichthyol /Noweda	Solutio Cordes®	138002	1
Ichthyol- Gesellschaft ...	Solutio Cordes®	13B001	1
Ichthyol Gesellschaft	Solutio Cordes®	14B006	1
Ichthyol Gesellschaft	Solutio Cordes®	14B012	1
Ichthyol Geselschaft Co...	Solutio Cordes®	18B004	1
Ichthyol/AHCA	Solutio Cordes®	17B007	1
Ichthyol/Ph	Solutio Cordes®	17B007	1
Ichthyol/Phönix	Solutio Cordes®	12B0005	1
Ichthyol/Phönix	Solutio Cordes®	12B005	15
Ichthyol/Phönix	Solutio Cordes®	13B002	3
Ichthyol/Phönix	Solutio Cordes®	14B011	1
Ichthyol/Phönix	Solutio Cordes®	15B001	1
Ichthyol/Phönix	Solutio Cordes®	20B0008	1
Ichthyol/Sanacorp	Solutio Cordes®	18B004	1
Ichthyol/Sanacorp	Solutio Cordes®	19B007	1
Ichthyol	Solutio Cordes®	12B005	1
Ichthyol	Solutio Cordes®	12B006	1
Ichthyol	Solutio Cordes®	13B001	1
Ichthyol	Solutio Cordes®	14B012	2
ichthyol	Solutio Cordes®	14B012	1
Ichthyol	Solutio Cordes®	15B005	1
ICHTHYOL	Solutio Cordes®	16B010	2
ichthyol	Solutio Cordes®	17B008	2
Ichthyol	Solutio Cordes®	18B004	1
Ichthyol	Solutio Cordes®	198004	1
ichthyol	Solutio Cordes®	19B005	1
Ichthyol	Solutio Cordes®	19007	1

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Supplier	Substance	Batch	Spectra
Ichthyolges.	Solutio Cordes®	17B007	5
Ichthyolges.	Solutio Cordes®	18B004	1
Ichthyol-Gesellschaft /...	Solutio Cordes®	18B004	1
Ichthyol-Gesellschaft /...	Solutio Cordes®	188004	1
Ichthyol-Gesellschaft C...	Solutio Cordes®	17B007	1
Ichthyol-Gesellschaft C...	Solutio Cordes®	18B004	1
Ichthyol-Gesellschaft C...	Solutio Cordes®	20B0008	1
Ichthyol-Gesellschaft/ ...	Solutio Cordes®	18B004	1
Ichthyol-Gesellschaft/ ...	Solutio Cordes®	18B004	1
Ichthyol-Gesellschaft	Solutio Cordes®	15B005	1
Ichthyol-Gesellschaft	Solutio Cordes®	18B004	1
Ichthyol-Gesellschaft	Solutio Cordes®	20B0008	1
Ichtyol	Solutio Cordes®	12B006	2
Ichtyol	Solutio Cordes®	13B002	1
Ichtyol-Gesellschaft Co...	Solutio Cordes®	18B004	1
Ichtyol-Gesellschaft/Ph...	Solutio Cordes®	200008	1
ICHTYOL-GESELLSCHAFT	Solutio Cordes®	13B001	1
Ichtyol-Gesellschaft	Solutio Cordes®	14B011	4
Ichtyol-Gesellschaft	Solutio Cordes®	15B001	2
Noweda	Solutio Cordes®	18B004	2
Phönix	Solutio Cordes®	13B002	1

- 15 340 spectra from 1163 *Apo-Ident* customers from a total of 4997 batches from a further 158 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 *Solutio Cordes*® 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 *Solutio Cordes*® 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	28 425
Type B	0	220	0	25 881
Type C	0	93	0	15 340

The substance/substance group *Solutio Cordes*® 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 % (> 99.9639 %)	100.0000 % (> 95.3846 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 98.9654 %)	100.0000 % (> 93.5484 %)

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

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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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Solutio Cordes*® in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Abitima® clinic body cream	67.01	–

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

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
30996	30996	0.00	75.31
31076	31076	0.00	76.36
35755	35755	0.00	83.59

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 2.5-2023-04

Validated substance/substance group	**Spearmint oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30453-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	1	5

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Spearmint oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 425 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 021 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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 5 batches from the substance/substance group *Spearmint oil*.
- 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
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

- 15 428 spectra from 1165 *Apo-Ident* customers from a total of 5019 batches from a further 158 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 *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	130	0	28 425
Type B	0	80	0	26 021
Type C	0	5	0	15 428

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 % (> 99.9639 %)	100.0000 % (> 95.3846 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9751 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Spearmint oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Pine silvestris oil	38.40	–
Juniper oil	43.60	–
Dwarf pine oil	48.14	–
Silver fir oil	49.52	–
Frankincense oil	53.99	–

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.

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	56.91
31685	31685	0.00	60.30
33481	33481	0.00	54.18

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Spruce needle oil / Pine silvestris oil / Frankincense oil / Silver**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	31032-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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

Calibration samples

Only spectra which have been recorded by *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
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 70 089 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.

- 27 675 spectra from a total of 585 batches from further 156 substances. These spectra were recorded by *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 by *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

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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

- 25 561 spectra from a total of 576 batches from further 206 substances. These spectra were recorded by *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.

- 41 spectra from 14 *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/Sanacorp	Spruce needle oil	11647-2942	1
Taoasis/Sanacorp	Spruce needle oil	534474-111869	1

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Supplier	Substance	Batch	Spectra
Taoasis/Sanacorp	Spruce needle oil	534474-113171	1
Taoasis	Spruce needle oil	114780-6023	1
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	1
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
Taoasis	Spruce needle oil	534474-111585	1
Taoasis	Frankincense oil	549702-112299	1
Taoasis	Silver fir oil	C100S-10426	2

- 15 392 spectra from 1165 *Apo-Ident* customers from a total of 4995 batches from a further 155 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	27 675
Type B	0	438	102	25 561
Type C	0	28	13	15 392

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 % (> 99.9635 %)	100.0000 % (> 99.3182 %)
Type B	100.0000 % (> 99.9508 %)	81.1111 % (> 80.5556 %)
Type C	100.0000 % (> 98.9661 %)	68.2927 % (> 60.9756 %)

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.)

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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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Spruce needle oil / Pine silvestris oil / Frankincense oil / Silver fir oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Swiss pine oil	11.36	–
Juniper oil	12.99	–
Spearmint oil	20.84	–
Dwarf pine oil	22.92	–
Angelica root oil	23.47	–
Ginger oil	28.80	–
Citus oil	29.69	–
Hyssop oil	30.03	–
Rosemary oil	31.16	–
Cypress oil	31.19	–
Marjoram oil	31.70	–
Citric oil	33.55	–
Lime oil	41.18	–
Myrtle oil	41.76	–
Sage oil	42.55	–
Cumin oil	49.43	–

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.

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	32.13
31255	31255	0.00	34.84
31633	31633	0.00	76.02
31754	31754	0.00	21.33
31819	31819	0.00	16.23
32066	32066	0.00	19.25
33052	33052	0.00	32.65
33646	33646	0.00	13.76
33650	33650	0.00	87.98

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33652	33652	0.00	85.97
33726	33726	0.00	11.62
33815	33815	0.00	15.05
34177	34177	0.00	19.71
34391	34391	0.00	29.96
37660	37660	0.00	18.06
37680	37680	0.00	83.12
37681	37681	0.00	26.08
37685	37685	0.00	11.36
37687	37687	0.00	18.31
37782	37782	0.00	30.03

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Stomahesive® adhesive paste**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30974-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Stomahesive® adhesive paste

Special notes

When selecting the *Stomahesive® adhesive paste* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Stomahesive® adhesive paste	3	2	5

Second-stage model

For differentiation of the substance/substance group *Stomahesive®* *adhesive paste* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Stomahesive®* *adhesive paste*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
ConvaTec Inc.	Stomahesive® adhesive paste	2D117	30974	80	not required
ConvaTec Inc.	Stomahesive® adhesive paste	2M084	31087	40	not required
ConvaTec Inc.	Stomahesive® adhesive paste	6L039	33474	40	not required

Validation samples

A total of 70 089 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 *Stomahesive®* *adhesive paste*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 395 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Stomahesive®* *adhesive paste*.
- 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
ConvaTec Inc.	Stomahesive® adhesive paste	6D079	32761	40
ConvaTec Inc.	Stomahesive® adhesive paste	5G062	32954	40

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- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.

- 30 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Stomahesive® adhesive paste*.
- 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
apomix	Stomahesive® adhesive paste	9B033	2
ConvaTec/ Alliance	Stomahesive® adhesive paste	9K007	2
Convatec/Gehe	Stomahesive® adhesive paste	9D046	1
Convatec/Phönix	Stomahesive® adhesive paste	6D079	1
Convatec	Stomahesive® adhesive paste	5G062	24

- 15 403 spectra from 1165 *Apo-Ident* customers from a total of 5019 batches from a further 158 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 *Stomahesive® adhesive paste* 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 *Stomahesive® adhesive paste* 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	28 395
Type B	0	80	0	26 021
Type C	0	30	0	15 403

The substance/substance group *Stomahesive® adhesive paste* 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 % (> 99.9638 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9665 %)	100.0000 % (> 80.0000 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Stomahesive®* *adhesive paste* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Lygal® ointment base	31.98	–
Lygal® head ointment N 3%	44.28	–
La Roche-Posay Cold Cream Naturel	105.71	–

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

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
30974	30974	0.00	53.17
31087	31087	0.00	56.27
33474	33474	0.00	56.87

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Strawberry aroma**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30643-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	47

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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.

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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

- 25 901 spectra from a total of 584 batches from further 209 substances. These spectra were recorded by *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.

- 172 spectra from 88 *Apo-Ident* customers from 49 batches from the substance/substance group *Strawberry aroma*.

- Among them are spectra of independent samples from 47 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	Strawberry aroma	10184917	1
Caelo	Strawberry aroma	10803202	1
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	5
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	4
Caelo	Strawberry aroma	192763001	2
Caelo	Strawberry aroma	192763002	5
Caelo	Strawberry aroma	192763004	2
Caelo	Strawberry aroma	192763005	5
Caelo	Strawberry aroma	192763008	3
Caelo	Strawberry aroma	192763009	3

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Supplier	Substance	Batch	Spectra
Caelo	Strawberry aroma	192763012	4
Caelo	Strawberry aroma	192763015	5
Caelo	Strawberry aroma	197263012	2
Caelo	Strawberry aroma	21002299001	4
Caelo	Strawberry aroma	21002299004	3
Caelo	Strawberry aroma	21002299007	1
Caelo	Strawberry aroma	21002299012	1
Caelo	Strawberry aroma	22002985001	2
Caelo	Strawberry aroma	70441927634	1
Caelo	Strawberry aroma	9101405	1
Caesar & Loretz GmbH / ...	Strawberry aroma	18083206	1
Caesar & Loretz GmbH/ A...	Strawberry aroma	18083206	1
Caesar & Loretz GmbH/ P...	Strawberry aroma	192763008	1
Caesar & Loretz GmbH/AHD	Strawberry aroma	192763008	1
Caesar & Loretz GmbH/Gehe	Strawberry aroma	192763016	1
Caesar & Loretz GmbH/Je...	Strawberry aroma	18083211	2
Caesar & Loretz GmbH/No...	Strawberry aroma	192763008	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	2
Caesar & Loretz GmbH	Strawberry aroma	21002299010	1
Caesar & Loretz GmbH	Strawberry aroma	21002299012	1
Caesar & Loretz GmbH	Strawberry aroma	22002985001	3
Caesar & Loretz GmbH	Strawberry aroma	22002985005	1
Caesar & Loretz GmbH	Strawberry aroma	22002985007	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
Hedinger	Strawberry aroma	14311215	1
Kehr	Strawberry aroma	21002299005	3
noweda	Strawberry aroma	192763002	1
Noweda	Strawberry aroma	21002299013	1
Sanacorp	Strawberry aroma	18083211	1

- 15 261 spectra from 1162 *Apo-Ident* customers from a total of 4975 batches from a further 158 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*).

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	False positive	True positive	False negative	True negative
Type A	0	200	0	28 355
Type B	0	200	0	25 901
Type C	0	172	0	15 261

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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 98.9651 %)	100.0000 % (> 96.5116 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Strawberry aroma* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Raspberry aroma	43.87	–
Contramarum aroma	86.44	–

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.

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	90.86
31395	31395	0.00	80.74
32814	32814	0.00	86.72
32838	32838	0.00	66.82
36891	36891	0.00	89.49

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Swiss pine oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31553-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	2	2

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 315 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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 *Swiss pine 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Primavera	Swiss pine oil	00661A27	34386	40
Taoasis	Swiss pine oil	201610159-126370	32793	40

- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 *Swiss pine 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	Swiss pine oil	6158653	1
Oswald	Swiss pine oil	9971217	1

- 15 431 spectra from 1165 *Apo-Ident* customers from a total of 5022 batches from a further 158 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	28 315
Type B	0	40	40	26 021
Type C	0	2	0	15 431

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 % (> 99.9637 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9511 %)	50.0000 % (> 46.2500 %)
Type C	100.0000 % (> 98.9905 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Swiss pine oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Silver fir oil	10.04	–
Frankincense oil	13.99	–
Dwarf pine oil	14.26	–
Pine silvestris oil	19.20	–
Cypress oil	19.58	–
Spruce needle oil	19.64	–
Angelica root oil	21.74	–
Spearmint oil	26.08	–
Juniper oil	28.17	–
Marjoram oil	29.97	–
Ginger oil	32.11	–
Citus oil	34.51	–

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.

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	20.90
31680	31680	0.00	14.31
32934	32934	0.00	24.49
33645	33645	0.00	17.68
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

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variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Tea tree oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30959-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	5	26

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Tea tree oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 28 415 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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

continued on the next page

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continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Tea tree oil	52642-125539	33017	40
Taoasis	Tea tree oil	52642-124527	33018	40
Taoasis	Tea tree oil	17186AUR08	37772	40

- 25 901 spectra from a total of 583 batches from further 209 substances. These spectra were recorded by *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.

- 45 spectra from 14 *Apo-Ident* customers from 26 batches from the substance/substance group *Tea tree 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
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
Ferd.Eimermacher GmbH	Tea tree oil	73900719	1
Taoasis/Taoasis	Tea tree oil	JF20461-1972	1
Taoasis	Tea tree oil	128919-AUJ07	1
Taoasis	Tea tree oil	1469-117418	2
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

- 15 388 spectra from 1165 *Apo-Ident* customers from a total of 4998 batches from a further 158 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	140	0	28 415
Type B	0	200	0	25 901
Type C	0	45	0	15 388

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 % (> 99.9639 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 98.9660 %)	100.0000 % (> 86.6667 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Tea tree oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Marjoram oil	21.73	–
Carrot seed oil	44.43	–
Patchouli oil	73.78	–

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.

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:

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30959	30959	0.00	51.68
31134	31134	0.00	53.64
31762	31762	0.00	59.14

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 2.5-2023-04

Validated substance/substance group	**Thuja oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	33828-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Thuja oil; Thuja (essential oil)

Special notes

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

- Advice: Currently no longer available. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Thuja oil	2	1	0

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Thuja oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Taoasis	Thuja oil	66255-969	33828	40	not required
Taoasis	Thuja oil	66255-2932	34287	40	not required

Validation samples

A total of 70 089 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 *Thuja oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 28 475 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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 *Thuja 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	Thuja oil	28508-121881	34038	40

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- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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 *Thuja 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.
- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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 *Thuja 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 *Thuja 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	28 475
Type B	0	40	0	26 061
Type C	0	0	0	15 433

The substance/substance group *Thuja 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 % (> 99.9642 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9514 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Thuja oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Cumin oil	45.38	–
Frankincense oil	52.44	–

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

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
33828	33828	0.00	44.27
34287	34287	0.00	47.30

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Thyme oil, red**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30929-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	1	24

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 295 spectra from a total of 598 batches from further 159 substances. These spectra were recorded by *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 by *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 *Thyme oil, red*.
- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Thyme oil, red	40517-121881	32472	40

- 26 061 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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.

- 32 spectra from 9 *Apo-Ident* customers from 25 batches from the substance/substance group *Thyme oil, red*.

- Among them are spectra of independent samples from 24 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	Thyme oil, red	19243015	1
Caelo	Thyme oil, red	21000083004	1
Caesar & Loretz GmbH	Thyme oil, red	5841	1
Noweda/ Taoasis 07.09.2...	Thyme oil, red	6164-10928	1
Noweda/Taoasis	Thyme oil, red	6164-12709	1
Taoasis/Sanacorp	Thyme oil, red	1976-3455	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
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	1
Taoasis	Thyme oil, red	56081-126921	1
Taoasis	Thyme oil, red	56081-127214	1
Taoasis	Thyme oil, red	9434-115525	1

- 15 401 spectra from 1165 *Apo-Ident* customers from a total of 4999 batches from a further 158 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	28 295
Type B	0	40	0	26 061
Type C	0	30	2	15 401

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 % (> 99.9637 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9514 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 98.9664 %)	93.7500 % (> 84.3750 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Thyme oil, red* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Savory herb	18.98	–
Oregano oil	22.21	–

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.

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:

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30929	30929	0.00	26.22
31259	31259	0.00	21.97
32482	32482	0.00	30.47
32981	32981	0.00	24.55
34103	34103	0.00	27.79
35537	35537	0.00	22.63

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 2.5-2023-04

Validated substance/substance group	**Thyme oil, white / Coriander oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31552-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Thyme oil, white / Coriander oil; Coriander oil; Oleum coriandri; Thyme oil, white

Special notes

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

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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, white / Coriander oil	9	6	14

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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, white / Coriander oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
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 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 400 spectra of 9 reference samples from the substance/substance group *Thyme oil, white / Coriander oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.
- 28 155 spectra from a total of 595 batches from further 158 substances. These spectra were recorded by *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 by *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 *Thyme oil, white / Coriander 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.

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Supplier	Substance	Batch	Sample ID	Spectra
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

- 25 861 spectra from a total of 582 batches from further 208 substances. These spectra were recorded by *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.

- 14 spectra from 14 *Apo-Ident* customers from 14 batches from the substance/substance group *Thyme oil, white / Coriander oil*.
- Among them are spectra of independent samples from 14 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 & Cie. ...	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
primavera	Thyme oil, white	334A2B	1
Primavera	Thyme oil, white	340L29	1
Sanacorp	Coriander oil	18125703	1
Taoasis GmbH	Thyme oil, white	114133-9219	1
taoasis	Coriander oil	104709127	1
Taoasis	Coriander oil	9291-1307	1

- 15 419 spectra from 1164 *Apo-Ident* customers from a total of 5010 batches from a further 157 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, white / Coriander 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 *Thyme oil, white / Coriander 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	400	0	28 155
Type B	0	239	1	25 861
Type C	0	13	1	15 419

The substance/substance group *Thyme oil, white / Coriander 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 % (> 99.9636 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9509 %)	99.5833 % (> 98.3333 %)
Type C	100.0000 % (> 98.9685 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Thyme oil, white / Coriander oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Basil oil	11.70	–
Matricaria oil, morrocan	18.65	–
Neroli oil	32.57	–
Rosewood oil	48.26	–
Carrot seed oil	49.90	–
Marjoram oil	60.66	–

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

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	12.32
31690	31690	0.00	11.70
32792	32792	0.00	42.43

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
33796	33796	0.00	34.95
33818	33818	0.00	13.12
34176	34176	0.00	35.94
34286	34286	0.00	33.08
37673	37673	0.00	17.29
37787	37787	0.00	40.61

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 2.5-2023-04

Validated substance/substance group	**Vetiver bourbon oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31546-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	4	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

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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 *Vetiver bourbon oil*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 28 355 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 26 021 spectra from a total of 587 batches from further 209 substances. These spectra were recorded by *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

- 15 418 spectra from 1165 *Apo-Ident* customers from a total of 5015 batches from a further 158 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	200	0	28 355
Type B	0	80	0	26 021
Type C	0	15	0	15 418

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 % (> 99.9637 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9511 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 98.9682 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Vetiver bourbon oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Citus oil	28.95	–
Myrtle oil	28.95	–
Cypress oil	29.40	–
Immortelle oil	30.14	–
Manuka oil	34.35	–
Rose-geranium oil, organic	35.66	–
Patchouli oil	36.84	–
Carrot seed oil	38.70	–
Ginger oil	38.98	–
Marjoram oil	39.01	–
Hyssop oil	42.57	–
Tea tree oil	46.79	–
Citronella oil	50.59	–

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.

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	32.33
31684	31684	0.00	30.67
33647	33647	0.00	30.70
35143	35143	0.00	36.17

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

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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 2.5-2023-04

Validated substance/substance group	**Wart ointment InfectoPharm® (NRF 11.31)**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	30730-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Wart ointment InfectoPharm® (NRF 11.31)

Special notes

When selecting the *Wart ointment InfectoPharm® (NRF 11.31)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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
Wart ointment InfectoPharm® (NRF 11.31)	3	4	58

Second-stage model

For differentiation of the substance/substance group *Wart ointment InfectoPharm® (NRF 11.31)* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 *Wart ointment InfectoPharm® (NRF 11.31)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Infectopharm	Wart ointment InfectoPharm® ...	S031201.1	30730	40	not required
Infectopharm	Wart ointment InfectoPharm® ...	S031201.1	30905	40	not required
Infectopharm	Wart ointment InfectoPharm® ...	S121103.1	30906	40	not required
Infectopharm	Wart ointment InfectoPharm® ...	S112001.1	35259	40	not required

Validation samples

A total of 70 089 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 *Wart ointment InfectoPharm® (NRF 11.31)*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

- 28 395 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Wart ointment InfectoPharm® (NRF 11.31)*.

- 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Infectopharm	Wart ointment InfectoPharm® ...	S021601.1	32593	40
Infectopharm	Wart ointment InfectoPharm® ...	S071602.1	32953	40
Infectopharm	Wart ointment InfectoPharm® ...	S061801.1	34517	40
Infectopharm	Wart ointment InfectoPharm® ...	S042201.1	36775	40
Infectopharm	Wart ointment InfectoPharm® ...	S071602.1	33515	40

- 25 901 spectra from a total of 584 batches from further 209 substances. These spectra were recorded by *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.

- 390 spectra from 172 *Apo-Ident* customers from 74 batches from the substance/substance group *Wart ointment InfectoPharm® (NRF 11.31)*.

- Among them are spectra of independent samples from 18 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	Wart ointment InfectoPharm® ...		1
Caelo	Wart ointment InfectoPharm® ...		5
Caelo	Wart ointment InfectoPharm® ...	s0617012	1
Caelo	Wart ointment InfectoPharm® ...	S111202	1
Eigenherstellung	Wart ointment InfectoPharm® ...		1
Euro OTC	Wart ointment InfectoPharm® ...		1
Fagron	Wart ointment InfectoPharm® ...		1
Fiebig/ Infectopharm	Wart ointment InfectoPharm® ...		1
Galderma/Phönix	Wart ointment InfectoPharm® ...		1
gehe/infecto	Wart ointment InfectoPharm® ...		1
Gehe	Wart ointment InfectoPharm® ...		2
GEHE	Wart ointment InfectoPharm® ...		3
GUMO	Wart ointment InfectoPharm® ...		1
Ichthyol-Gesellschaft C...	Wart ointment InfectoPharm® ...		1
Ichthyolgesellschaft/Gehe	Wart ointment InfectoPharm® ...		1
Ichthyol-Gesellschaft/N...	Wart ointment InfectoPharm® ...		1
Infec/ Phönix	Wart ointment InfectoPharm® ...		1
Infect/PX	Wart ointment InfectoPharm® ...		2
infectipharm/Phönix	Wart ointment InfectoPharm® ...		1
Infecto Pharm / Noweda	Wart ointment InfectoPharm® ...		4
Infecto Pharm	Wart ointment InfectoPharm® ...		3
Infecto Pharma /Sanacorp	Wart ointment InfectoPharm® ...		2
Infecto/Gehe	Wart ointment InfectoPharm® ...		1
infecto/Phönix	Wart ointment InfectoPharm® ...		1
Infecto/Spangro	Wart ointment InfectoPharm® ...		1
Infectoph./Gehe	Wart ointment InfectoPharm® ...		1
Infectoph./Kehr	Wart ointment InfectoPharm® ...		2
Infectopharm (Phoenix)	Wart ointment InfectoPharm® ...		1
Infectopharm / Alliance...	Wart ointment InfectoPharm® ...		1
InfectoPharm / Alliance...	Wart ointment InfectoPharm® ...		2
Infectopharm / Alliance	Wart ointment InfectoPharm® ...		1
Infectopharm / Gehe	Wart ointment InfectoPharm® ...		3
InfectoPharm / Gehe	Wart ointment InfectoPharm® ...		1

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Supplier	Substance	Batch	Spectra
Infectopharm / Noweda	Wart ointment InfectoPharm® ...		1
Infectopharm / Phoenix	Wart ointment InfectoPharm® ...		1
Infectopharm / Phönix	Wart ointment InfectoPharm® ...		1
InfectoPharm / Phönix	Wart ointment InfectoPharm® ...		1
Infectopharm / Phönix	Wart ointment InfectoPharm® ...	3718A-03898	1
Infectopharm / Phönix	Wart ointment InfectoPharm® ...	4117A-03898	1
Infectopharm / Sanacorp	Wart ointment InfectoPharm® ...		1
InfectoPharm / Sanacorp	Wart ointment InfectoPharm® ...		1
Infectopharm Arzneimitt...	Wart ointment InfectoPharm® ...		1
Infectopharm Arzneimittel	Wart ointment InfectoPharm® ...		18
InfectoPharm GmbH	Wart ointment InfectoPharm® ...		1
Infectopharm GmbH	Wart ointment InfectoPharm® ...	s061801-1	1
INFECTOPHARM -Noweda	Wart ointment InfectoPharm® ...		1
Infectopharm Sanacorp	Wart ointment InfectoPharm® ...	S061801	1
Infectopharm/ Alliance	Wart ointment InfectoPharm® ...		1
InfectoPharm/ E	Wart ointment InfectoPharm® ...		1
InfectoPharm/ Gehe	Wart ointment InfectoPharm® ...		2
Infectopharm/ Jenne	Wart ointment InfectoPharm® ...		2
Infectopharm/ Now	Wart ointment InfectoPharm® ...		1
Infectopharm/ Noweda	Wart ointment InfectoPharm® ...		3
InfectoPharm/ Noweda	Wart ointment InfectoPharm® ...		2
InfectoPharm/ Phoenix/ ...	Wart ointment InfectoPharm® ...		2
Infectopharm/ Phönix	Wart ointment InfectoPharm® ...		1
Infectopharm/ Sanacorp	Wart ointment InfectoPharm® ...		2
Infectopharm/	Wart ointment InfectoPharm® ...		1
Infectopharm/AEP	Wart ointment InfectoPharm® ...		1
Infectopharm/AEP	Wart ointment InfectoPharm® ...	S112001	1
Infectopharm/AHD	Wart ointment InfectoPharm® ...		1
InfectoPharm/AHD	Wart ointment InfectoPharm® ...		1
Infectopharm/AHD	Wart ointment InfectoPharm® ...	S1219021	1
Infectopharm/Alliance H...	Wart ointment InfectoPharm® ...		1
infectopharm/Alliance	Wart ointment InfectoPharm® ...		2
Infectopharm/AllianceHe...	Wart ointment InfectoPharm® ...		1
Infectopharm/Allianz	Wart ointment InfectoPharm® ...		4
Infectopharm/Anzag 08.0...	Wart ointment InfectoPharm® ...		1
Infectopharm/Anzag	Wart ointment InfectoPharm® ...		2
InfectoPharm/Anzag	Wart ointment InfectoPharm® ...		2
InfectoPharm/Anzag	Wart ointment InfectoPharm® ...	716A-03898	1
Infectopharm/Ebert	Wart ointment InfectoPharm® ...		1
InfectoPharm/Fiebig	Wart ointment InfectoPharm® ...		1
Infectopharm/G	Wart ointment InfectoPharm® ...		1
INFECTOPHARM/GEHE 02.05...	Wart ointment InfectoPharm® ...		1
INFECTOPHARM/GEHE 07.07...	Wart ointment InfectoPharm® ...		1
INFECTOPHARM/GEHE 28.09...	Wart ointment InfectoPharm® ...		1
Infectopharm/Gehe	Wart ointment InfectoPharm® ...		28
Infectopharm/GEHE	Wart ointment InfectoPharm® ...		4
InfectoPharm/Gehe	Wart ointment InfectoPharm® ...		3
InfectoPharm/GEHE	Wart ointment InfectoPharm® ...		1
Infectopharm/Jenne	Wart ointment InfectoPharm® ...		2
InfectoPharm/Jenne	Wart ointment InfectoPharm® ...		1
Infectopharm/K	Wart ointment InfectoPharm® ...		1
Infectopharm/Kehr	Wart ointment InfectoPharm® ...		1
InfectoPharm/Krieger	Wart ointment InfectoPharm® ...		2
Infectopharm/Nk	Wart ointment InfectoPharm® ...		1
Infectopharm/Nk	Wart ointment InfectoPharm® ...	S051901	1
Infectopharm/Noweda	Wart ointment InfectoPharm® ...		19
InfectoPharm/Noweda	Wart ointment InfectoPharm® ...		4
Infectopharm/Noweda	Wart ointment InfectoPharm® ...	S0521011	1
Infectopharm/Noweda	Wart ointment InfectoPharm® ...	S0716021	1
Infectopharm/Phoenix Le...	Wart ointment InfectoPharm® ...		1

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Supplier	Substance	Batch	Spectra
Infectopharm/Phoenix	Wart ointment InfectoPharm® ...		8
InfectoPharm/Phoenix	Wart ointment InfectoPharm® ...		8
infectopharm/Phönix	Wart ointment InfectoPharm® ...		1
Infectopharm/Phönix	Wart ointment InfectoPharm® ...		12
InfectoPharm/Phönix	Wart ointment InfectoPharm® ...		1
Infectopharm/Römer/Noweda	Wart ointment InfectoPharm® ...	S0215011	2
Infectopharm/Sanacorp	Wart ointment InfectoPharm® ...		1
InfectoPharm/Sanacorp	Wart ointment InfectoPharm® ...		2
Infectopharm/Spangro	Wart ointment InfectoPharm® ...	S061801-1	1
infectopharm	Wart ointment InfectoPharm® ...		4
Infectopharm	Wart ointment InfectoPharm® ...		70
InfectoPharm	Wart ointment InfectoPharm® ...		23
Infectopharm	Wart ointment InfectoPharm® ...	3013I-07003	1
infectopharm	Wart ointment InfectoPharm® ...	S0211604	1
InfectoPharm	Wart ointment InfectoPharm® ...	S0215011	1
Infectopharm	Wart ointment InfectoPharm® ...	S041301	1
InfectoPharm	Wart ointment InfectoPharm® ...	s061801	1
Infectopharm	Wart ointment InfectoPharm® ...	S111202	1
Infectopharma	Wart ointment InfectoPharm® ...		1
InfectoPharma	Wart ointment InfectoPharm® ...		1
InfectopharmNoweda	Wart ointment InfectoPharm® ...		1
Infectophsrm	Wart ointment InfectoPharm® ...		1
InfektoPharm GmbH / Ph...	Wart ointment InfectoPharm® ...		1
Jenne / Infectopharm	Wart ointment InfectoPharm® ...		4
Löwen City-Apotheke Bar...	Wart ointment InfectoPharm® ...	8032013	1
Nachprüfung	Wart ointment InfectoPharm® ...		1
nfectoPharm	Wart ointment InfectoPharm® ...		1
Noweda/ Infectopharm	Wart ointment InfectoPharm® ...		10
Noweda/Infecto Pharma	Wart ointment InfectoPharm® ...		1
Noweda/infectopharm	Wart ointment InfectoPharm® ...		1
Noweda/Infectopharm	Wart ointment InfectoPharm® ...		2
Noweda/InfectoPharm	Wart ointment InfectoPharm® ...		6
Noweda	Wart ointment InfectoPharm® ...		2
Phoenix	Wart ointment InfectoPharm® ...		4
Phönix Gotha	Wart ointment InfectoPharm® ...		1
Phönix, Infectopharm,03...	Wart ointment InfectoPharm® ...	S129021	1
Phönix/ Infectopharm	Wart ointment InfectoPharm® ...		2
Phönix/InfectoPharm/ 15...	Wart ointment InfectoPharm® ...		1
Phönix/Infectopharm	Wart ointment InfectoPharm® ...		1
PX/Infectop	Wart ointment InfectoPharm® ...	S0215011	3
Sana/ Infectopharm	Wart ointment InfectoPharm® ...		1
Sanacorp / Infectopharm	Wart ointment InfectoPharm® ...		1
Sanacorp/Infectopharm	Wart ointment InfectoPharm® ...		1
Sanacorp	Wart ointment InfectoPharm® ...		4
Spangropharm	Wart ointment InfectoPharm® ...		1

- 15 043 spectra from 1156 *Apo-Ident* customers from a total of 4951 batches from a further 158 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 *Wart ointment InfectoPharm® (NRF 11.31)* 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

Wart ointment InfectoPharm® (NRF 11.31) 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	28 395
Type B	0	200	0	25 901
Type C	0	390	0	15 043

The substance/substance group *Wart ointment InfectoPharm® (NRF 11.31)* 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 % (> 99.9638 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9509 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 98.9649 %)	100.0000 % (> 98.4615 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Wart ointment InfectoPharm® (NRF 11.31)* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Salicylic white paraffin 10%	127.60	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Wart ointment InfectoPharm® (NRF 11.31)* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

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
30730	30730	0.00	213.33
30905	30905	0.00	212.23
30906	30906	0.00	212.37
35259	35259	0.00	199.60

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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 2.5-2023-04

Validated substance/substance group	**Water and aqueous solutions**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`10005444-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Water and aqueous solutions; Aloe vera gel, 1:1; 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 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	26	71	401

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

Calibration samples

Only spectra which have been recorded by *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, 1:1	13025802	31145	40	not required
Caelo	Aloe vera gel, 1:1	15329203	31866	60	not required
Caelo	Aloe vera gel, 1:1	153292	31880	60	20151111*
Caelo	Aloe vera gel, 1:1	153292	31881	60	20151111*
Caelo	Aloe vera gel, 1:1	21002409	35604	50	20210830*
Caelo	Aloe vera gel, 1:1	22001060	36257	40	20220407*
Caelo	Aloe vera gel, 1:1	22002254	36469	40	20220722*
Caelo	Aloe vera gel, 10x concentra…	13045901	31146	40	not required
Caelo	Aloe vera gel, 10x concentra…	15185503	31862	60	not required
Caelo	Aloe vera gel, 10x concentra…	161922	32313	40	20160707*
Caelo	Aloe vera gel, 10x concentra…	20001962	35049	40	20200702*
Retterspitz G…	Retterspitz external	016100	32785	40	not required
Retterspitz G…	Retterspitz external	017058	33430	40	not required
Retterspitz G…	Retterspitz external	016240	33431	40	not required
Fagron	SyrSpend® SF pH4 cherry aroma	1503D017	31671	60	not required
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	2H11-T10-099025	36745	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 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1315 spectra of 28 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 26 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.

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- 27 240 spectra from a total of 578 batches from further 154 substances. These spectra were recorded by *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 by *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.

- 2595 spectra of 74 reference samples from the substance/substance group *Water and aqueous solutions*.

- Among them are spectra of independent samples from 71 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	Aloe vera gel, 1:1	162489	32580	40
Caelo	Aloe vera gel, 1:1	162912	32899	40
Caelo	Aloe vera gel, 1:1	171341	33411	40
Caelo	Aloe vera gel, 1:1	172891	33736	40
Caelo	Aloe vera gel, 1:1	172890	33970	40
Caelo	Aloe vera gel, 1:1	181943	34251	40
Caelo	Aloe vera gel, 1:1	191914	34764	40
Caelo	Aloe vera gel, 1:1	23000170	36915	40
Caelo	Aloe vera gel, 1:1	23001282	37471	40
Caelo	Aloe vera gel, 10x concentra…	17082002	33511	40
Caelo	Aloe vera gel, 10x concentra…	181255	34342	40
Caelo	Aloe vera gel, 10x concentra…	192411	34714	40
Caelo	Aloe vera gel, 10x concentra…	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

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Supplier	Substance	Batch	Sample ID	Spectra
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
Caelo	Water	23000974	37473	10
Caelo	Water	23000975	37707	10
Caelo	Aloe vera gel, 1:1	23000170	36916	10
Fagron	SyrSpend® SF pH4 aroma free	1704493	33631	40
Caelo	Water	15068701	31675†	15

- 23 506 spectra from a total of 516 batches from further 204 substances. These spectra were recorded by *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.

- 1987 spectra from 454 *Apo-Ident* customers from 415 batches from the substance/substance group *Water and aqueous solutions*.

†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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- Among them are spectra of independent samples from 398 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 cherry aroma	21010483	1
	SyrSpend® SF pH4 cherry aroma	22C13-T06-103720	1
	SyrSpend® SF pH4 cherry aroma	22D11-T17-095910	1
	SyrSpend® SF pH4 cherry aroma	22D11-T18-095918	1
	SyrSpend® SF pH4 aroma free	22h11-t09	1
	SyrSpend® SF pH4 aroma free	22h11-t09-099022	1
	SyrSpend® SF pH4 cherry aroma	23A26-T03-102457	2
	SyrSpend® SF pH4 cherry aroma	23a26-to3-102457	1
	SyrSpend® SF pH4 aroma free	23B10-T02	1
	SyrSpend® SF pH4 aroma free	23b10-t02-102920	1
	SyrSpend® SF pH4 aroma free	23B10-T02-102920	1
	SyrSpend® SF pH4 aroma free	23b17-t03-103125	1
	SyrSpend® SF pH4 aroma free	23B17-T03-103125	2
	SyrSpend® SF pH4 cherry aroma	23c08-t04-103682	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
Anzag	SyrSpend® SF pH4 aroma free	19011410	1
Anzag	SyrSpend® SF pH4 aroma free	20004220	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	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 concentra...	15185503	1
Caelo	Aloe vera gel, 10x concentra...	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
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	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

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Supplier	Substance	Batch	Spectra
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	Aloe vera gel, 1:1	17289003	2
Caelo	Aloe vera gel, 1:1	17289101	2
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	1806233/2P-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	Aloe vera gel, 1:1	18194304	3
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	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
Caelo	SyrSpend® SF pH4 aroma free	1906126	2
Caelo	Aloe vera gel, 10x concentra…	19066601	2
Caelo	Aloe vera gel, 1:1	19069002	1
Caelo	Aloe vera gel, 1:1	19069003	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, 1:1	19191401	6
Caelo	Aloe vera gel, 10x concentra…	19241101	1
Caelo	Water	19246201	1
Caelo	Aloe vera gel, 1:1	19255202	1
Caelo	Aloe vera gel, 10x concentra…	19255203	1
Caelo	Aloe vera gel, 1:1	19255204	1
Caelo	Aloe vera gel, 1:1	20000289003	7
Caelo	Water	20000526002	1
Caelo	Water	20001119001	1

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Supplier	Substance	Batch	Spectra
Caelo	Water	20002379002	1
Caelo	Aloe vera gel, 1:1	20002878005	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	Aloe vera gel, 1:1	21001591003	1
Caelo	Aloe vera gel, 1:1	21002409001	1
Caelo	Aloe vera gel, 1:1	21002409002	4
Caelo	SyrSpend® SF pH4 cherry aroma	21002532	2
Caelo	Water	21003422001	1
Caelo	Water	219181	1
Caelo	SyrSpend® SF pH4 cherry aroma	22D11-T17-095910	1
Caelo	Water	LOTAP0041	1
Caelo	Water	LOTAP0078	1
Caelo	Water	LOTAP-SP0001	1
Caesar & Loretz GmbH / …	Water	16127901	1
Caesar & Loretz GmbH/Ph…	Aloe vera gel, 1:1	21002409002	2
Caesar & Loretz GmbH	Aloe vera gel, 10x concentra…	18125504	1
Caesar & Loretz GmbH	SyrSpend® SF pH4 cherry aroma	19000779004	1
Caesar & Loretz GmbH	Aloe vera gel, 1:1	19191401	1
Caesar & Loretz GmbH	Aloe vera gel, 10x concentra…	192411002	1
Caesar & Loretz GmbH	Aloe vera gel, 10x concentra…	19241101	1
Caesar & Loretz GmbH	Aloe vera gel, 10x concentra…	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	Aloe vera gel, 1:1	22001060004	1
Caesar & Loretz GmbH	Aloe vera gel, 1:1	22002254002	1
Caesar & Loretz GmbH	Aloe vera gel, 1:1	22002254004	1
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
Fagron	SyrSpend® SF pH4 aroma free		3
Fagron	SyrSpend® SF pH4 aroma free	102653/1	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
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

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Supplier	Substance	Batch	Spectra
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	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	17E05T07044067	1
Fagron	Water	17E05T11044076	1
Fagron	Water	17E05-T13-044080	1
Fagron	Water	17F23-T06-045760	1
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

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Supplier	Substance	Batch	Spectra
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	1804245/1	25
Fagron	SyrSpend® SF pH4 aroma free	1804245/2	2
Fagron	SyrSpend® SF pH4 aroma free	1804245-2	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	1808206/1	3
Fagron	SyrSpend® SF pH4 aroma free	1808206/12	1
Fagron	SyrSpend® SF pH4 aroma free	1808206/2	61
Fagron	SyrSpend® SF pH4 aroma free	1808206/2A	1
Fagron	SyrSpend® SF pH4 aroma free	1808206/2B	1
Fagron	SyrSpend® SF pH4 aroma free	1808206-2	1
Fagron	SyrSpend® SF pH4 aroma free	1812150/2	15
Fagron	SyrSpend® SF pH4 aroma free	1814231	29
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	18C19T31054017	1
Fagron	Water	18C19-T31-054017	2
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
Fagron	Water	18G16-T04-058129	2
Fagron	Water	18G16-T05-058132	1
Fagron	Water	18L19To6o62853	1
Fagron	SyrSpend® SF pH4 cherry aroma	1900093	27
Fagron	SyrSpend® SF pH4 cherry aroma	19009673	1
Fagron	SyrSpend® SF pH4 aroma free	19011410	68
Fagron	SyrSpend® SF pH4 aroma free	190114110	1
Fagron	SyrSpend® SF pH4 cherry aroma	1904383	1
Fagron	SyrSpend® SF pH4 aroma free	1906126	31
Fagron	SyrSpend® SF pH4 aroma free	1907122	22
Fagron	SyrSpend® SF pH4 cherry aroma	1908041	1
Fagron	SyrSpend® SF pH4 cherry aroma	19094223/2	1
Fagron	SyrSpend® SF pH4 cherry aroma	1909423/1	15
Fagron	SyrSpend® SF pH4 cherry aroma	1909423/2	2
Fagron	SyrSpend® SF pH4 cherry aroma	1909423-2	1
Fagron	SyrSpend® SF pH4 cherry aroma	1909673	51
Fagron	SyrSpend® SF pH4 cherry aroma	190973	1
Fagron	SyrSpend® SF pH4 aroma free	1911010	5
Fagron	SyrSpend® SF pH4 aroma free	19911010	1

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Supplier	Substance	Batch	Spectra
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	76
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	40
Fagron	SyrSpend® SF pH4 aroma free	20004220	10
Fagron	SyrSpend® SF pH4 cherry aroma	20004221	13
Fagron	SyrSpend® SF pH4 cherry aroma	20004332	46
Fagron	SyrSpend® SF pH4 cherry aroma	20004369	3
Fagron	SyrSpend® SF pH4 cherry aroma	200047312	1
Fagron	SyrSpend® SF pH4 aroma free	20006608	28
Fagron	SyrSpend® SF pH4 cherry aroma	20006936	19
Fagron	SyrSpend® SF pH4 cherry aroma	20007125	33
Fagron	SyrSpend® SF pH4 cherry aroma	20007130	6
Fagron	SyrSpend® SF pH4 cherry aroma	20007312	58
Fagron	SyrSpend® SF pH4 cherry aroma	20007312mfa	1
Fagron	SyrSpend® SF pH4 cherry aroma	20007317	15
Fagron	SyrSpend® SF pH4 aroma free	20007563	12
Fagron	SyrSpend® SF pH4 aroma free	20007575	7
Fagron	SyrSpend® SF pH4 aroma free	20009273	20
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
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	43
Fagron	SyrSpend® SF pH4 aroma free	21005761	4
Fagron	SyrSpend® SF pH4 aroma free	21009136	15
Fagron	SyrSpend® SF pH4 cherry aroma	21010483	22
Fagron	Water	21G28-T25-090471	1
Fagron	SyrSpend® SF pH4 aroma free	22000887	7
Fagron	SyrSpend® SF pH4 aroma free	22092007	1
Fagron	SyrSpend® SF pH4 aroma free	22092008	2
Fagron	SyrSpend® SF pH4 aroma free	22D11-T08	1
Fagron	SyrSpend® SF pH4 aroma free	22D11-T08-095894	1
Fagron	SyrSpend® SF pH4 aroma free	22D11T09	1
Fagron	SyrSpend® SF pH4 aroma free	22D11-T09-095898	8
Fagron	SyrSpend® SF pH4 cherry aroma	22D11-T17-095910	9
Fagron	SyrSpend® SF pH4 cherry aroma	22D11-T17-095911	1
Fagron	SyrSpend® SF pH4 cherry aroma	22D11-T18-095918	1
Fagron	SyrSpend® SF pH4 aroma free	22H11-165220	1
Fagron	SyrSpend® SF pH4 aroma free	22H11-T09-099022	6
Fagron	SyrSpend® SF pH4 aroma free	22H11T10099025	1
Fagron	SyrSpend® SF pH4 aroma free	22H11-T10-099025	1

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Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF pH4 cherry aroma	22H11-T11-099029	6
Fagron	SyrSpend® SF pH4 cherry aroma	22H11-T11-099030	3
Fagron	SyrSpend® SF pH4 cherry aroma	22H11-T13	1
Fagron	SyrSpend® SF pH4 cherry aroma	22H11-T13-099034	4
Fagron	SyrSpend® SF pH4 cherry aroma	22H11-T13-099035	1
Fagron	SyrSpend® SF pH4 cherry aroma	22H11-T17-095910	2
Fagron	SyrSpend® SF pH4 cherry aroma	22H11-T18	1
Fagron	SyrSpend® SF pH4 cherry aroma	22H11-T18-099038	7
Fagron	SyrSpend® SF pH4 cherry aroma	22H30-T05-099074	1
Fagron	SyrSpend® SF pH4 cherry aroma	22J14-T08-100064	7
Fagron	SyrSpend® SF pH4 cherry aroma	22J14-T08-100065	1
Fagron	SyrSpend® SF pH4 cherry aroma	22J14-T08	1
Fagron	SyrSpend® SF pH4 cherry aroma	23A05-T07-102866	2
Fagron	SyrSpend® SF pH4 cherry aroma	23A26-T03-102457	2
Fagron	SyrSpend® SF pH4 aroma free	27121704	1
Fagron	SyrSpend® SF pH4 cherry aroma	2x1712024	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 aroma free	T09-0958909	1
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	2
Fagron	SyrSpend® SF pH4 aroma free	T08-0958904	1
Fagron	SyrSpend® SF pH4 aroma free	T09-0958908	1
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	SyrSpend® SF pH4 cherry aroma	1900093	1
Fargon	SyrSpend® SF pH4 cherry aroma	1909673	2
Fargron/Phönix	Water	18C19-T31-054017	1
Fargron/PNACH	SyrSpend® SF pH4 aroma free	1712023/1	1
Fgron / Kehr 03.02.2020	SyrSpend® SF pH4 aroma free	1812150/2	1
Fiebig/Fagon	SyrSpend® SF pH4 cherry aroma	20004332	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
Fragron	SyrSpend® SF pH4 cherry aroma	1702015	1
Fresenius /Noweda	Water	19KK24GA	1
GEHE	Water	17114801	1
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	5
Gehe	SyrSpend® SF pH4 aroma free	1812150/2	2
Gehe	SyrSpend® SF pH4 aroma free	1814231	3
Gehe	SyrSpend® SF pH4 aroma free	19011410	4
Gehe	SyrSpend® SF pH4 aroma free	1906126	1
Gehe	SyrSpend® SF pH4 cherry aroma	1909423/1	1

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Supplier	Substance	Batch	Spectra
Gehe	SyrSpend® SF pH4 cherry aroma	1909673	1
Gehe	SyrSpend® SF pH4 aroma free	20004219	1
Gehe	SyrSpend® SF pH4 aroma free	20006608	3
Gehe	SyrSpend® SF pH4 cherry aroma	20007152	1
Gehe	SyrSpend® SF pH4 cherry aroma	21002532	2
GEHE	SyrSpend® SF pH4 cherry aroma	22H11-T18-099038	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/Noweda	Water	219209	6
Hedinger/Noweda	Water	219212	9
Hedinger/Phoenix	Water	219206	4
Hedinger/Phoenix	Water	219222	6
Hedinger/Phoenix	Water	219227	1
Hedinger	Water	219140	1
HEDINGER	Water	219162	1
Hedinger	Water	219208	1
HEDINGER	Water	LOTAP0071	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
Ichthyol/Gehe	SyrSpend® SF pH4 cherry aroma	1900093	1
Jenne	SyrSpend® SF pH4 cherry aroma	1900093	2
Kehr.21.07.2020	SyrSpend® SF pH4 cherry aroma	20000326	1
Kehr.26.03.2020	SyrSpend® SF pH4 aroma free	1814231	1
Kehr	SyrSpend® SF pH4 cherry aroma	23A10-T20-102143	1
kerndl-Noweda	Water		2
Krieger	SyrSpend® SF pH4 aroma free	20004219	2
L30	Water	17291301	1
Lamotte	Aloe vera gel, 1:1	19191403	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
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	Aloe vera gel, 1:1	17289003	1
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 cherry aroma	21010483	1
Phoenix	Water	15L14-T14-028664	1
Phoenix	Aloe vera gel, 1:1	17134105	1
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

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Supplier	Substance	Batch	Spectra
Phoenix	Water	3387	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&Loretz G...	SyrSpend® SF pH4 cherry aroma	20004332	1
Phönix/Fagro GmbH&Co.KG...	SyrSpend® SF pH4 aroma free	20004219	1
Phönix	SyrSpend® SF pH4 cherry aroma		1
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 aroma free	20009273	2
Phönix	Water	LOTAP0154	1
Resana/Phönix	Aloe vera gel, 10x concentra...	1901-6285	1
Retterspitz/ Phoenix	Retterspitz external	17224	1
Retterspitz/ Phoenix	Retterspitz external	18045	1
Sanacorp/Wepa	Water	LOTAP-SP0003	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	1
Sanacorp	SyrSpend® SF pH4 aroma free	20004219	2
Sanacorp	SyrSpend® SF pH4 aroma free	20009273	4
Sanacorp	SyrSpend® SF pH4 aroma free	22000887	1
serumwerk bernburg - Gehe	Water		5
Serumwerk Bernburg AG	Water		1
Serumwerk Bernburg	Water		1
Spinnrad	Aloe vera gel, 10x concentra...	319502021	1
Tiofarma B.V.	SyrSpend® SF pH4 aroma free	1410D020	1
Walter Schmidt Chemie G...	Water	95058	1
Wepa / Sanacorp	Water	LotAP0088	1
WEPA Apothekenbedarf Gm...	Water	LOTAP0158	1
WEPA Apothekenbedarf Gm...	Water	LOTAP0095	1
Wepa Apothekenbedarf	Water	LOTAP0050	1
Wepa Phönix	Water	LOTAPSP0003	1
Wepa/ Wepa	Water	LOTAP0077	1
Wepa/AHCA	Water	LOTAP0099	1
WEPA/Krieger	Water	LOTAP0086	1
Wepa/Wepa/ 13.05.2019/ ...	Water	LOTAP0101	1
Wepa/Wepa	Water	LOTAP0037	1
WEPA/WEPA	Water	LOTAP0088	1
Wepa/Wepa	Water	LOTAP0112	1
Wepa/Wepa	Water	LOTAP-SP0023	1
wepa	Water	AP00036	1
Wepa	Water	AP0072	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

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Supplier	Substance	Batch	Spectra
Wepa	Water	LOTAP0084	1
Wepa	Water	LOTAP0087	1
Wepa	Water	LOTAP0123	1
Wepa	Water	LOTAP0144	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

- 13 446 spectra from 1120 *Apo-Ident* customers from a total of 4610 batches from a further 153 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	1315	0	27 240
Type B	0	2594	1	23 106
Type C	0	1910	77	13 431

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 % (> 99.9635 %)	100.0000 % (> 99.5437 %)
Type B	100.0000 % (> 99.9508 %)	99.9615 % (> 99.8459 %)
Type C	100.0000 % (> 98.9661 %)	96.1248 % (> 95.9738 %)

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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Water and aqueous solutions* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

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Substance	Distance in main model	Distance in second-stage model
Fenistil® Gel	14.36	–
Sebexol® cream lotion pH 5	20.54	–
Sebexol® basic pH 5 formula basis	27.06	–
Excipial® U Hydrolotio	31.64	–
Wofacutan wash lotion	31.81	–
Hans Karrer Hydrocream MicroSilver	33.40	–
Dimeticone ointment 10% SR	34.69	–
Abitima® clinic face cream	45.88	–
Amciderm® Base cream	47.30	–
Hans Karrer Lipolotion MicroSilver	68.20	–

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.

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
31145	31145	0.00	29.96
31146	31146	0.00	28.29
31623	31623	0.00	30.45
31670	31670	0.00	29.19
31671	31671	0.00	29.80
31675	31675	0.00	32.38
31722	31722	0.00	28.71
31723	31723	0.00	28.75
31862	31862	0.00	28.05
31866	31866	0.00	30.92
31880	31880	0.00	31.68
31881	31881	0.00	30.83
32079	32079	0.00	30.92
32313	32313	0.00	27.75
32785	32785	0.00	18.75
33430	33430	0.00	24.81
33431	33431	0.00	25.09
33787	33787	0.00	28.02
34767	34767	0.00	31.48
35049	35049	0.00	24.66
35077	35077	0.00	27.91
35239	35239	0.00	31.00
35240	35240	0.00	30.78
35242	35242	0.00	30.60
35604	35604	0.00	31.32
36257	36257	0.00	31.11
36469	36469	0.00	31.75
36745	36745	0.00	28.49

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Wax ointment (stabilised)**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31111-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Wax ointment (stabilised); Unguentum cereum

Special notes

When selecting the *Wax ointment (stabilised)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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 (stabilised)	6	12	92

Second-stage model

For differentiation of the substance/substance group *Wax ointment (stabilised)* the following second-stage model is used:

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 (stabilised)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Wax ointment (stabilised)	13072102	31111	40	not required
Caelo	Wax ointment (stabilised)	13307701	31167	40	not required
Caelo	Wax ointment (stabilised)	14073701	31444	40	not required
Caelo	Wax ointment (stabilised)	154243	31911	60	20151217*
Caelo	Wax ointment (stabilised)	154244	31912	60	20151217*
Caelo	Wax ointment (stabilised)	22001707	36402	40	20220705*

Validation samples

A total of 70 089 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 (stabilised)*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 28 275 spectra from a total of 598 batches from further 159 substances. These spectra were recorded by *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 by *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.

- 450 spectra of 12 reference samples from the substance/substance group *Wax ointment (stabilised)*.

*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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- 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
Caelo	Wax ointment (stabilised)	12352501	30967	40
Caelo	Wax ointment (stabilised)	161215	32117	40
Caelo	Wax ointment (stabilised)	161334	32118	40
Caelo	Wax ointment (stabilised)	171714	33550	40
Caelo	Wax ointment (stabilised)	172942	34024	40
Caelo	Wax ointment (stabilised)	191905	34793	40
Caelo	Wax ointment (stabilised)	19000784	34984	40
Caelo	Wax ointment (stabilised)	20002322	35095	40
Caelo	Wax ointment (stabilised)	21003702	35985	40
Caelo	Wax ointment (stabilised)	22002672	36652	40
Caelo	Wax ointment (stabilised)	23000483	36971	40
Caelo	Wax ointment (stabilised)	23000484	36972	10

- 25 651 spectra from a total of 576 batches from further 209 substances. These spectra were recorded by *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.

- 769 spectra from 271 *Apo-Ident* customers from 95 batches from the substance/substance group *Wax ointment (stabilised)*.

- Among them are spectra of independent samples from 92 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 (stabilised)	22002672001	1
AHD	Wax ointment (stabilised)	14073701	1
Alliance Healthcare	Wax ointment (stabilised)	18162202	1
Alliance Healthcare	Wax ointment (stabilised)	19190502	2
Anzag 07.12.12	Wax ointment (stabilised)	12128702	1
Caello/Phönix	Wax ointment (stabilised)	16121501	2
Caelo	Wax ointment (stabilised)	1000337003	1
Caelo	Wax ointment (stabilised)	1021303	1
Caelo	Wax ointment (stabilised)	1114E3212	1
Caelo	Wax ointment (stabilised)	11321302	1
Caelo	Wax ointment (stabilised)	11355201	2
Caelo	Wax ointment (stabilised)	11355202	1
Caelo	Wax ointment (stabilised)	12033602	2
Caelo	Wax ointment (stabilised)	12033701	3
Caelo	Wax ointment (stabilised)	1218702	2
Caelo	Wax ointment (stabilised)	12209401	3
Caelo	Wax ointment (stabilised)	12209402	1
Caelo	Wax ointment (stabilised)	12352051	1
Caelo	Wax ointment (stabilised)	12352501	4
Caelo	Wax ointment (stabilised)	12378701	5
Caelo	Wax ointment (stabilised)	13072102	13

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Supplier	Substance	Batch	Spectra
Caelo	Wax ointment (stabilised)	13159302	7
Caelo	Wax ointment (stabilised)	13159303	2
Caelo	Wax ointment (stabilised)	13307701	17
Caelo	Wax ointment (stabilised)	13307802	13
Caelo	Wax ointment (stabilised)	14072801	1
Caelo	Wax ointment (stabilised)	1407301	1
Caelo	Wax ointment (stabilised)	14073701	15
Caelo	Wax ointment (stabilised)	140737012	1
Caelo	Wax ointment (stabilised)	140737701	1
Caelo	Wax ointment (stabilised)	14073801	7
Caelo	Wax ointment (stabilised)	14073802	1
Caelo	Wax ointment (stabilised)	14235901	13
Caelo	Wax ointment (stabilised)	14236001	3
Caelo	Wax ointment (stabilised)	14236002	4
Caelo	Wax ointment (stabilised)	14236003	1
Caelo	Wax ointment (stabilised)	15025701	1
Caelo	Wax ointment (stabilised)	15025702	11
Caelo	Wax ointment (stabilised)	15025801	17
Caelo	Wax ointment (stabilised)	15205402	13
Caelo	Wax ointment (stabilised)	1524301	1
Caelo	Wax ointment (stabilised)	1524401	1
Caelo	Wax ointment (stabilised)	15424301	19
Caelo	Wax ointment (stabilised)	15424401	9
Caelo	Wax ointment (stabilised)	15424402	4
Caelo	Wax ointment (stabilised)	16121501	8
Caelo	Wax ointment (stabilised)	16121502	4
Caelo	Wax ointment (stabilised)	16133401	22
Caelo	Wax ointment (stabilised)	17014901	27
Caelo	Wax ointment (stabilised)	17015001	20
Caelo	Wax ointment (stabilised)	17015002	1
Caelo	Wax ointment (stabilised)	17171401	20
Caelo	Wax ointment (stabilised)	17294201	21
Caelo	Wax ointment (stabilised)	17294202	16
Caelo	Wax ointment (stabilised)	18034601	3
Caelo	Wax ointment (stabilised)	18034602	21
Caelo	Wax ointment (stabilised)	18162201	7
Caelo	Wax ointment (stabilised)	18162202	14
Caelo	Wax ointment (stabilised)	18258501	28
Caelo	Wax ointment (stabilised)	19000783001	33
Caelo	Wax ointment (stabilised)	19000784001	6
Caelo	Wax ointment (stabilised)	19000784002	11
Caelo	Wax ointment (stabilised)	19040001	10
Caelo	Wax ointment (stabilised)	19040002	23
Caelo	Wax ointment (stabilised)	19040003	5
Caelo	Wax ointment (stabilised)	19190501	29
Caelo	Wax ointment (stabilised)	19190502	3
Caelo	Wax ointment (stabilised)	200003013002	1
Caelo	Wax ointment (stabilised)	20002187004	1
Caelo	Wax ointment (stabilised)	20002322002	14
Caelo	Wax ointment (stabilised)	20003013001	8
Caelo	Wax ointment (stabilised)	20003013002	6
Caelo	Wax ointment (stabilised)	20051012-1	1
Caelo	Wax ointment (stabilised)	20121305	1
Caelo	Wax ointment (stabilised)	21000337001	2
Caelo	Wax ointment (stabilised)	21000337002	12
Caelo	Wax ointment (stabilised)	21000337003	1
Caelo	Wax ointment (stabilised)	21000337225	1
Caelo	Wax ointment (stabilised)	2100259002	1
Caelo	Wax ointment (stabilised)	21002596001	6
Caelo	Wax ointment (stabilised)	21002596002	2

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Supplier	Substance	Batch	Spectra
Caelo	Wax ointment (stabilised)	21002596003	1
Caelo	Wax ointment (stabilised)	21003702001	3
Caelo	Wax ointment (stabilised)	21003702002	1
Caelo	Wax ointment (stabilised)	21003702003	3
Caelo	Wax ointment (stabilised)	2113Q-03212	1
Caelo	Wax ointment (stabilised)	22001707001	1
Caelo	Wax ointment (stabilised)	22001707003	1
Caelo	Wax ointment (stabilised)	22002672001	1
Caelo	Wax ointment (stabilised)	220204A	1
Caelo	Wax ointment (stabilised)	23000484001	1
Caelo	Wax ointment (stabilised)	270120-01	1
Caelo	Wax ointment (stabilised)	28051511	1
Caelo	Wax ointment (stabilised)	3427	1
Caelo	Wax ointment (stabilised)	7071204	1
Caelo	Wax ointment (stabilised)	9531609	1
Caelo	Wax ointment (stabilised)	U-150513-2	1
Caeol/Noweda	Wax ointment (stabilised)	17294201	1
Caeol/Phoenix	Wax ointment (stabilised)	15424301	1
Caesar & Loretz GmbH/ A…	Wax ointment (stabilised)	19040002	1
Caesar & Loretz GmbH/ N…	Wax ointment (stabilised)	21002596001	1
Caesar & Loretz GmbH/ O…	Wax ointment (stabilised)	19000783001	1
Caesar & Loretz GmbH/Fi…	Wax ointment (stabilised)	19190501	1
Caesar & Loretz GmbH/Gehe	Wax ointment (stabilised)	19000783001	1
Caesar & Loretz GmbH/Gehe	Wax ointment (stabilised)	20002322001	2
Caesar & Loretz GmbH/Gehe	Wax ointment (stabilised)	20003013002	1
Caesar & Loretz GmbH/Je…	Wax ointment (stabilised)	19040002	1
Caesar & Loretz GmbH/Je…	Wax ointment (stabilised)	21000337002	1
Caesar & Loretz GmbH/Kehr	Wax ointment (stabilised)	19000783001	1
Caesar & Loretz GmbH/Kr…	Wax ointment (stabilised)	19000783001	1
Caesar & Loretz GmbH/Kr…	Wax ointment (stabilised)	21000337002	1
Caesar & Loretz GmbH/No…	Wax ointment (stabilised)	19000783001	1
Caesar & Loretz GmbH/No…	Wax ointment (stabilised)	20002322001	1
Caesar & Loretz GmbH/Ph…	Wax ointment (stabilised)	19040002	1
Caesar & Loretz GmbH/Ph…	Wax ointment (stabilised)	19190501	2
Caesar & Loretz GmbH/Ph…	Wax ointment (stabilised)	190007840	1
Caesar & Loretz GmbH/Ph…	Wax ointment (stabilised)	19040001	2
Caesar & Loretz GmbH/Ph…	Wax ointment (stabilised)	19040002	1
Caesar & Loretz GmbH/Sa…	Wax ointment (stabilised)	19000784002	3
Caesar & Loretz GmbH/Sa…	Wax ointment (stabilised)	20002322002	1
Caesar & Loretz GmbH	Wax ointment (stabilised)	13072102	1
Caesar & Loretz GmbH	Wax ointment (stabilised)	18162202	2
Caesar & Loretz GmbH	Wax ointment (stabilised)	18258501	7
Caesar & Loretz GmbH	Wax ointment (stabilised)	19000783001	8
Caesar & Loretz GmbH	Wax ointment (stabilised)	19000784002	3
Caesar & Loretz GmbH	Wax ointment (stabilised)	19040001	4
Caesar & Loretz GmbH	Wax ointment (stabilised)	19040002	3
Caesar & Loretz GmbH	Wax ointment (stabilised)	19190501	10
Caesar & Loretz GmbH	Wax ointment (stabilised)	19190502	7
Caesar & Loretz GmbH	Wax ointment (stabilised)	20002322001	2
Caesar & Loretz GmbH	Wax ointment (stabilised)	20002322002	8
Caesar & Loretz GmbH	Wax ointment (stabilised)	20003013002	5
Caesar & Loretz GmbH	Wax ointment (stabilised)	21000337001	2
Caesar & Loretz GmbH	Wax ointment (stabilised)	21000337002	6
Caesar & Loretz GmbH	Wax ointment (stabilised)	21002596001	7
Caesar & Loretz GmbH	Wax ointment (stabilised)	21003702003	3
Caesar & Loretz GmbH	Wax ointment (stabilised)	22002672001	1
Caesar und Loretz GmbH	Wax ointment (stabilised)	17015001	1
Caesar& Loretz GmbH	Wax ointment (stabilised)	21002596002	1
Cealo / Otto Geilenkirc…	Wax ointment (stabilised)	19000783001	1
Cealo/Noweda	Wax ointment (stabilised)	16133401	1

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Supplier	Substance	Batch	Spectra
Cealo/Noweda	Wax ointment (stabilised)	19190501	1
Cealo/Sanacorp	Wax ointment (stabilised)	18034602	1
Cealo	Wax ointment (stabilised)	19190501	1
Celo	Wax ointment (stabilised)	15424402	1
Gehe	Wax ointment (stabilised)	13072102	1
Gehe	Wax ointment (stabilised)	14235901	1
Gehe	Wax ointment (stabilised)	16133401	1
GEHE	Wax ointment (stabilised)	17171401	1
Gehe	Wax ointment (stabilised)	20002322002	1
Gehe	Wax ointment (stabilised)	20003013002	3
Hedinger GmbH &Co KG	Wax ointment (stabilised)	18034602	1
Henry Lamotte Olis GmbH…	Wax ointment (stabilised)	15424301	1
Jenne	Wax ointment (stabilised)	19000783001	1
Noweda	Wax ointment (stabilised)	17171401	1
Noweda	Wax ointment (stabilised)	19040002	1
Noweda	Wax ointment (stabilised)	19190501	1
Pharmachem/Sanacorp	Wax ointment (stabilised)	18L18-To9-062847	2
Phoenix	Wax ointment (stabilised)	19000783001	1
Phoenix	Wax ointment (stabilised)	19000784002	3
Phönix	Wax ointment (stabilised)	18258501	1
Sanacoro W.E:06.03.18 …	Wax ointment (stabilised)	17171401	1
Sanacorp	Wax ointment (stabilised)	12352501	1
Sanacorp	Wax ointment (stabilised)	14073701	1
Sanacorp	Wax ointment (stabilised)	15205402	2
Sanacorp	Wax ointment (stabilised)	17015001	1
Sanacorp	Wax ointment (stabilised)	17294202	1
Sanacorp	Wax ointment (stabilised)	18162202	4
VDL;6,45EUR;21.10.14	Wax ointment (stabilised)	14235901	1

- 14 664 spectra from 1149 *Apo-Ident* customers from a total of 4929 batches from a further 158 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 (stabilised)* 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 (stabilised)* 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	28 275
Type B	0	450	0	25 651
Type C	0	768	1	14 664

The substance/substance group *Wax ointment (stabilised)* 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 % (> 99.9637 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9508 %)	100.0000 % (> 98.6667 %)
Type C	100.0000 % (> 98.9649 %)	99.8700 % (> 99.4798 %)

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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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Wax ointment (stabilised)* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Cottonwood ointment	18.07	–
Marjoram ointment	22.25	–
Neribas® fat ointment	26.37	–
Protegin® XN	31.93	–
Deumavan® protection ointment neutral	34.05	–
Excipial® almond oil ointment	37.24	–
White paraffin oil	40.01	–
Balm Bio Nature	41.08	–
Salicylic white paraffin 10%	42.40	–
Argan oil	45.71	–
Lygal® ointment base	54.39	–

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

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	33.47
31167	31167	0.00	37.08
31444	31444	0.00	32.99
31911	31911	0.00	29.97
31912	31912	0.00	36.44
36402	36402	0.00	31.43

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**White paraffin oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`32342-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	2	17

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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

Validation samples

A total of 70 089 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.
- 28 395 spectra from a total of 600 batches from further 159 substances. These spectra were recorded by *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 by *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 *White paraffin 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.

*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	White paraffin oil	14338604	32454	40
Caelo	White paraffin oil	21004217002	36584	40
Caelo	White paraffin oil	14338604	32846	40

- 25 981 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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 20 *Apo-Ident* customers from 17 batches from the substance/substance group *White paraffin 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
Caelo	White paraffin oil	16219207	1
Caelo	White paraffin oil	17175501	2
Caelo	White paraffin oil	17175506	2
Caelo	White paraffin oil	17175509	1
Caelo	White paraffin oil	18226101	1
Caelo	White paraffin oil	18226104	1
Caelo	White paraffin oil	18226105	1
Caelo	White paraffin oil	190763002	1
Caelo	White paraffin oil	19076301	2
Caelo	White paraffin oil	19076302	2
Caelo	White paraffin oil	20002135004	1
Caelo	White paraffin oil	20004223002	3
Caelo	White paraffin oil	21004217002	1
Caesar & Loretz GmbH/ A...	White paraffin oil	21004217002	1
Caesar & Loretz GmbH/No...	White paraffin oil	18226105	1
Caesar & Loretz GmbH	White paraffin oil	17175509	1
Caesar & Loretz GmbH	White paraffin oil	20004223002	1
Caesar & Loretz GmbH	White paraffin oil	21001958002	1
Caesar & Loretz GmbH	White paraffin oil	21002439002	1
Cealo / Spangro	White paraffin oil	16219204	1
Hänseler	White paraffin oil		1

- 15 406 spectra from 1165 *Apo-Ident* customers from a total of 5007 batches from a further 158 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	28 395
Type B	0	120	0	25 981
Type C	0	27	0	15 406

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 % (> 99.9638 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9667 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *White paraffin oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Deumavan® protection ointment neutral	10.55	–
Marjoram ointment	20.66	–
Neribas® fat ointment	21.96	–
Cottonwood ointment	23.94	–
Protegin® XN	26.09	–
Asche Basis® fat ointment	29.22	–
Wax ointment (stabilised)	40.46	–
Lygal® head ointment N 3%	41.41	–
Lygal® ointment base	46.64	–

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.

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:

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
32342	32342	0.00	15.20
32565	32565	0.00	17.48
35598	35598	0.00	19.75
37454	37454	0.00	18.39

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 2.5-2023-04

Validated substance/substance group	**Wintergreen oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`30455-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	12

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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	56	not required
Taoasis	Wintergreen oil	1828-125286	32807	40	not required

Validation samples

A total of 70 089 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 96 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.
- 28 459 spectra from a total of 602 batches from further 159 substances. These spectra were recorded by *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 by *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

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- 25 941 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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 11 *Apo-Ident* customers from 13 batches from the substance/substance group *Wintergreen oil*.

- Among them are spectra of independent samples from 12 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	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	Wintergreen oil	200D28	1
Taoasis/Taoasis	Wintergreen oil	2387-7212	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

- 15 420 spectra from 1165 *Apo-Ident* customers from a total of 5011 batches from a further 158 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	96	0	28 459
Type B	0	159	1	25 941
Type C	0	12	1	15 420

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 % (> 99.9640 %)	100.0000 % (> 93.7500 %)
Type B	100.0000 % (> 99.9509 %)	99.3750 % (> 97.5000 %)
Type C	100.0000 % (> 98.9688 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Wintergreen oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Clove oil	268.21	–

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.

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	283.97
32807	32807	0.00	284.76

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Yarrow oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	33795-2023-11-08
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	3	0

Second-stage model

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

no second-stage model

Calibration samples

Only spectra which have been recorded by *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 70 089 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.
- 28 435 spectra from a total of 601 batches from further 159 substances. These spectra were recorded by *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 by *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 *Yarrow 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	Yarrow oil	00677E26	34174	40
Primavera	Yarrow oil	00197J26	34295	40
Taoasis	Yarrow oil	128700	33823	40

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- 25 981 spectra from a total of 585 batches from further 209 substances. These spectra were recorded by *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.

- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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	28 435
Type B	0	120	0	25 981
Type C	0	0	0	15 433

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 % (> 99.9639 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9510 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Yarrow oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Citus oil	20.66	–
Myrtle oil	21.24	–
Marjoram oil	23.62	–
Hyssop oil	25.13	–
Angelica root oil	32.40	–
Cypress oil	35.87	–
Frankincense oil	35.88	–
Matricaria oil, morrocan	37.89	–
Rosemary oil	39.16	–
Spearmint oil	41.88	–
Ravensara oil	44.00	–
Juniper oil	45.38	–
Sage oil	46.15	–
Dwarf pine oil	47.14	–
Niaouli oil	50.07	–

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.

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	50.97
33822	33822	0.00	21.15
37650	37650	0.00	51.26

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.

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VALIDATION REPORT

IdentModule 2.5-2023-04

Validated substance/substance group	**Ylang-ylang oil**
Substance class	APIs & excipients, liquid/semi-solid (other)
Report date	08/11/2023
Report number	`31506-2023-11-08`
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 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

978-3-7692-7517-9	*European Pharmacopoeia 10th Edition, Basic Version 2020* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-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	2	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

Calibration samples

Only spectra which have been recorded by *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 70 089 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.

- 28 315 spectra from a total of 599 batches from further 159 substances. These spectra were recorded by *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 by *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 *Ylang-ylang 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.

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Supplier	Substance	Batch	Sample ID	Spectra
Taoasis	Ylang-ylang oil	43197-126348	33049	40
Taoasis	Ylang-ylang oil	B966015-128199	33648	40

- 26 021 spectra from a total of 586 batches from further 209 substances. These spectra were recorded by *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.
- 15 433 spectra from 1165 *Apo-Ident* customers from a total of 5024 batches from a further 159 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	28 315
Type B	0	40	40	26 021
Type C	0	0	0	15 433

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 % (> 99.9637 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9511 %)	50.0000 % (> 46.2500 %)
Type C	100.0000 % (> 98.9837 %)	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.

Nearest chemometric neighbours

The following table lists the closest chemometric neighbours of the substance/substance group *Ylang-ylang oil* in the substance class *APIs & excipients, liquid/semi-solid (other)*. Furthermore, their *Mahalanobis distance* is specified within the main model and, where appropriate, within the second-stage model.

Substance	Distance in main model	Distance in second-stage model
Clary sage oil	34.86	–
Petitgrain oil	48.15	–
Lavender oil	63.75	–

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.

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	85.33
31653	31653	0.00	36.06
32808	32808	0.00	73.36
34382	34382	0.00	67.63
37675	37675	0.00	89.72

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.

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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 by *HiperScan GmbH*.

The samples originate from 2 batches. From these, 90 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.

Supplier	Substance	Batch	Spectra	Certificate
Licca Klinik ...	Licca base ointment	HR1310926	50	not required
Ichthyol	Milk Cordes® O/W Emulsion	21D0006	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 by *HiperScan GmbH*. They are allocated to the *Type B*. They also include the calibration spectra for other models.

The samples originate from 119 batches. From these 5050 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.

Supplier	Substance	Batch	Spectra	Certificate
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
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
Dr. Wolff	Anefug® Simplex	234280	40	not required
Dr. Wolff	Anefug® Simplex	237590	40	1407216
Primavera	Anise seed oil	00480L26	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
Taoasis	Black cumin oil	504511-115611	40	not required
Koko	dermaviduals® base gel	L003L13	60	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
Primavera	Douglas fir oil	00539M26	40	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
Pharmapol	Glycerol trinitrate 5%	228718	40	not required
Pharmapol	Glycerol trinitrate 5%	232961	60	not required
Primavera	Ho leaf oil	00388M26	40	not required
Primavera	Jasmine 4% in alcohol	00184A27	40	not required
Spirig Pharma	Kerasal® base ointment	M031	40	not required
Spirig Pharma	Kerasal® base ointment	N011	40	not required

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Supplier	Substance	Batch	Spectra	Certificate
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® 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
Primavera	Litsea oil	00496L26	40	not required
Ichthyol	Milk Cordes® O/W Emulsion	22D0014	40	not required
Caelo	Milking grease Special without Osmaron®	162049	40	20160711*
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
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
Einhorn-Apoth...	Rizol raw material	AL0413-1	60	not required
Primavera	Rose oil 10%	00721716	40	not required
Salderman Gmb...	Salderman base emulsion	180123	40	not required
Salderman Gmb...	Salderman base emulsion	220321-1	40	not required
Primavera	Seabuckthorn oil, organic	00346E26	40	not required
Primavera	Spanish sage oil	00057G26	40	not required
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

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Supplier	Substance	Batch	Spectra	Certificate
Bene	Thrombocid® ointment	410B113	40	not required
Bene	Thrombocid® ointment	408C141	40	not required
Bene	Thrombocid® ointment	409A151	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
Bayer	Ultrabas®	33851A	40	not required
Hecht Pharma ...	Ultrabas®	34069	40	not required
Bayer	Ultraphil®	22100A	40	not required
Bayer	Ultrasicc®	33614A	40	not required
Hecht Pharma ...	Ultrasicc®	34837	40	not required
Caelo	Ultrasound contact gel	12031301	40	not required
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™	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

*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 253 batches. From these, 483 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.

Supplier	Substance	Batch	Spectra
Actavis/Alliance	Abitima® clinic body lotion	161613	1
Allergika Pharma GmbH	ALLERGIKA® – Base cream		1
allergika pharma gmbH...	ALLERGIKA® – Base cream	8/072024	1
Allergika Pharma/Sana...	ALLERGIKA® – Base cream	2012023	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
Dr. Wolff	Anefug® Simplex	136840	1

Supplier	Substance	Batch	Spectra
Fischar	Bepanthen® solution	6317104	1
Caelo	Bepanthen® solution	KV02S8P	1
Liechtenstein	Bepanthen® solution	2300380R	1

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

Supplier	Substance	Batch	Spectra
Allergika/Kehr	Dermifant® kids lotion	1604060	1
Sanacorp EK:10,80 ...	Dermifant® kids lotion	1705111	1

Supplier	Substance	Batch	Spectra
Fagron	Fitalite™	1503259	2

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	10
Pharmapol	Glycerol trinitrate 5%	228718	11

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Supplier	Substance	Batch	Spectra
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%	232961	6
Arzneimitte...			
Pharmapol/Zentrum Apo	Glycerol trinitrate 5%	2913A-07002	1

Supplier	Substance	Batch	Spectra
Anzag/Galderma	Kerasal® base ointment	S075	1
Galderma/Gehe	Kerasal® base ointment	S061	1
Galdermna/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

Supplier	Substance	Batch	Spectra
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	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 GmbH...	Linola® fat cream	6901	1
Dr. August Wolff/Phönix	Linola® fat cream	902800	1
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
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 / Alliance ...	Linola® fat cream	709800	1
Dr. Wolff / Gehe	Linola® fat cream	337860	1
Dr. Wolff /Anzag	Linola® fat cream	237710	1
Dr. Wolff 03.12.2013F...	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

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Supplier	Substance	Batch	Spectra
Dr. Wolff/Phönix	Linola® fat cream	810170	2
Dr.August Wolff Gmbh&...	Linola® fat cream	710080	2
Dr.August Wolff Gmbh&...	Linola® fat cream	810180	5
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	907080	5
Dr.Wolff	Linola® fat cream	6401	1
Dr.Wolff	Linola® fat cream	6410	2
Dr.Wolff	Linola® fat cream	143640	2
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-Apotheke B...	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/Phöenix	Linola® fat cream	807620	1
Wollf/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 GmbH...	Linola® O/W cream		2
Dr. August Wolff GmbH...	Linola® O/W cream	144790	1
Dr. August Wolff GmbH...	Linola® O/W cream	170522LC/701090	1
Dr. August Wolff GmbH...	Linola® O/W cream	808420	5
Dr. August Wolff GmbH...	Linola® O/W cream	901150	9
Dr. August Wolff GmbH...	Linola® O/W cream	908930	6
Dr. August Wolff GmbH...	Linola® O/W cream	904890	5
Dr. August Wolff GmbH...	Linola® O/W cream	1750	1
Dr. August Wolff/Sana...	Linola® O/W cream	807360	2

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Supplier	Substance	Batch	Spectra
Dr. August Wolff/Sana...	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 25.03.2013...	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 GmbH&...	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
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

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Supplier	Substance	Batch	Spectra
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
Noweda	Linola® O/W cream	90115	1
Noweda	Linola® O/W cream	3380	1
Noweda	Linola® O/W cream	7060	7
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

Supplier	Substance	Batch	Spectra
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
Ichtyol, Noweda	Milk Cordes® O/W Emulsion	13d007	1

Supplier	Substance	Batch	Spectra
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

Supplier	Substance	Batch	Spectra
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

Supplier	Substance	Batch	Spectra
Dyckerhoff	Regeneresen	60611dü-2	1
Dyckerhoff	Regeneresen	150173th-2	1
Dyckerhoff	Regeneresen	120292Ov-2	1
Dyckerhoff	Regeneresen	120323Lu-2	1
Dyckerhoff	Regeneresen	120313Kn-2	1
Dyckerhoff	Regeneresen	1503839-Na	1
Dyckerhoff	Regeneresen	120333NN-2	1

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Supplier	Substance	Batch	Spectra
Dyckerhoff	Regeneresen	120053NNR-2	1
Arkeo Immun UG	Rizol raw material	1192HJ	2
Caelo	Rizol raw material	15144304	1
Steidl/Phytolab	Rizol raw material	200812174102290	1

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

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

Supplier	Substance	Batch	Spectra
Taoasis	Wild rose oil	99149-99474	1
Taoasis	Wild rose oil	106177-106175	1

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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).

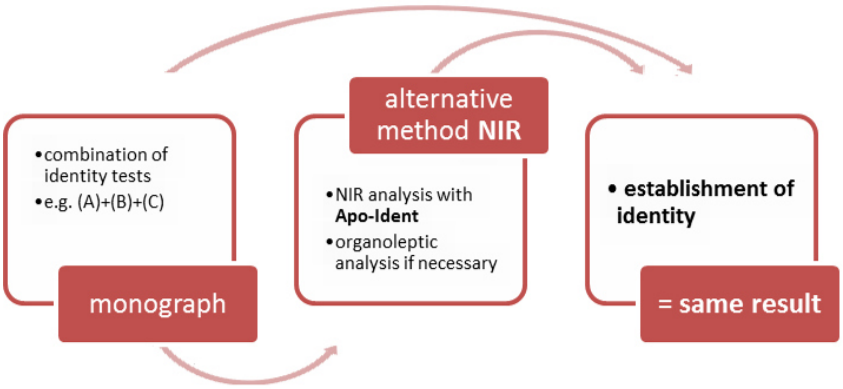

Figure 2: The combination of tests of the monograph is replaced by the alternative method NIR spectroscopy using *Apo-Ident*. This is permissible because both test procedures result in the establishment of the identity of the raw material.

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].

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