

Validation documentation
*APIs & excipients, liquid/semi-solid (with analysis
certificate)*

HiperScan GmbH

July 4, 2017

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Introduction

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

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

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

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

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

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

Context of this document

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

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

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.

Validity scope of this document

This validation documentation describes the results of the validation of the reference database for the substance class *APIs & excipients, liquid/semi-solid (with analysis certificate)*. 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 database is exclusively established from spectra which have been recorded by *HiperScan GmbH* for 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.
 - In three separately evaluated validation runs, calibration spectra, spectra from independent samples and spectra from independent field samples (described further below as *Type A*, *B* or *C*) are presented to the *IdentModule* for evaluation.
 - 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*).
- For each individual substance, the unambiguous identifiability with *Apo-Ident* and the demarkation against all other database substances is proven.

Validation concept

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

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

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

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

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

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

Model creation procedure and validation runs

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

1. Collecting the reference spectra (calibration sample)

- a) Procurement of the samples from the same sources from which pharmacies source their raw material for compounding (Caelo, Fagron, Euro-OTC, ..., see also *DAC III.2. Bezugsquellen-nachweis für Rezepturbestandteile* [Sources of supply for compounding] [7]).
- b) Testing the suitability according to *ApBetrO* [Pharmacies Rules and Regulations] §§ 6, 11, that is to say the availability of a valid manufacturer certificates via identity, purity and contents of the batch.
- c) Recording standard 40 spectra of the sample in different positions, as a standard on four instruments. Here, handling and presentation of the samples as later in the pharmacy.
- d) Visual checking for anomalies in the spectra. In case of indications of measurement errors, measurement must be repeated. If a signature is missing in the spectrum, the substance may be excluded from the start as not promising (the spectra are nonetheless entered in the database validation as independent *Type B* spectra).

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

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

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

2. Generating the chemometric models (calibration)

- a) Determination of the transformation matrix from the reference spectra using variance maximisation [8, 9]. (All reference spectra are always included, even if only a few spectra are added for an update.) All reference spectra receive the same data pre-treatment, which is also later applied to all measurement spectra in the field (in the pharmacies).
- b) Checking that the number of principal components used is still sufficient.
- c) Calculating the limits for each substance from the spread of the reference spectra. The calculation regulation is identical for each substance in a substance class.
- d) Checking the distances between the limits of the separable substances: the distance matrix incorporates the *Mahalanobis distances* from each substance to all the others. If a distance is less than 10, both two substances must be declared as inseparable or *both two* must be removed from the database. (The spectra of removed substances remain as independent *Type B* spectra in the validation.)
- e) Testing the model based on the reference spectra. If *false positive* results arise, you must proceed as in the case of *Mahalanobis distances* which are too small.
- f) If chemometric models are available for all substance classes which meet both criteria (distance matrix and no *false positives*), they are joined together with the evaluation algorithms as an *IdentModule* and encrypted. This unit can no longer be changed. Its overall function is tested by validation.

3. Set of validation spectra (validation samples)

The following is provided for validation:

- a) *Type A*: The reference spectra = calibration spectra from which the database was established. 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 from independent samples not included in the generation of the respective model received but were measured by *HiperScan GmbH*. These also include reference spectra from other substance classes and spectra which are not declared as reference spectra.
- c) *Type C*: Spectra from independent field samples. These measurements were recorded under normal everyday conditions by pharmacy staff. The spectra belong both to substances of the substance class to be examined and to substances from different classes.

All manufacturers' batches from which spectra flow into the validation are listed by substance in this document: for substances included in the substance class *APIs & excipients, liquid/semi-solid (with analysis certificate)* in the respective validation reports; otherwise in attachments [A](#), [B](#) and [C](#).

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

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

4. Validation runs and approval

- a) Validation spectra are transferred holistically to the *IdentModule* for evaluation in the same way as the spectroscopy software *QuickStep* transfers measured spectra.
- b) Following the provision of each spectrum, the *IdentModule* responds as to whether it has recognised a substance and which substance was recognised.
- c) The correctness of this response is checked for each possible initial assumption (each measurable substance with the substance class) and counted according to [true negative](#), [false negative](#), [true positive](#) and [false positive](#). These figures are provided for each substance and additionally in the section [Summary](#), separated according to types *A*, *B* and *C*.
- d) No *false positive* results whatsoever are permissible.
- e) If the criterion is also met for all substance classes, the *IdentModule* is approved.

Particularities of individual substance classes

Basically, *HiperScan GmbH* procures and tests the manufacturer's certificate for the batch, commissions external testing of the identity of the sample or carries it out independently and stores the certificates. As described, this process is established for the Pharmacopoeia substances, that is to say for substance classes *APIs & excipients, solid*, *APIs & excipients, liquid/semi-solid (with analysis certificate)*, *Narcotic substances, liquid/semi-solid* and *Drugs*. 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.

Also, the substance classes with **TCM – Granulated herbal extracts** are separated supplier-specifically. The granulates from the suppliers *HerbaSinica*, *PhytoComm* and *China-Medica* are hardly comparable with each other due to their spectra, because extracts of respectively different drug batches with different carrier materials are granulated. The spectra for all batches from these suppliers are recorded by *HiperScan GmbH* and entered in the respective database. The suppliers organise the respective tests themselves and keep the test certificates. The process implemented with *HerbaSinica*

is a particularity: The reference samples are sent to a test laboratory which determines the identity of the sample and sends the container to *HiperScan GmbH* if the result is positive.

A new evaluation option was created for the class *TCM – Granulated herbal extracts (PhytoComm)* with the update 2016-01. As the risks are considerably fewer than those from chemical agents, the pharmacist can specify a reasonable criterion for the *specificity* in accordance with internal risk estimation. The database for this is created without taking safety distances into account and no criterion is determined in advance for the *specificity*. Instead, the *specificity* for testing the identity with this concrete substance is calculated in the validation for each substance and provided with the measurement result. The pharmacist then judges himself whether this safety is reasonable with regard to the risk of the substance.

Additionally, a statistical forecast is provided for the *specificity* which is determined according to the *Rule of Three* [10, 11]. For this forecast, it is assumed that there would have been three wrong results more and is provided with a lower limit for *specificity*. This value has a special meaning if a *specificity* of 100 % is achieved for a substance during validation. In this case, the lower limit allows conclusions regarding the scale of existing safety for which with an endless number of validation spectra a value of less than 100 % is to be assumed.

If, for example 14000 spectra not belonging to the substance are presented and no *false positive* classification is made, a hypothetical number of three *false positive* results is assumed (*Rule of Three* [10, 11]) and the *specificity* is defined with 100.0000 % (> 99.9786 %). Here, it applies that the higher the number of validation spectra which form the statistical basis, the better the *specificity* calculated via the lower *specificity* limit will be approximated.

The positive result of the identity test using *Apo-Ident* establishes that the sample spectrum is in accordance with a batch of the specified granulate from this supplier, whereby all useable batches from the supplier are known.

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

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

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

Conclusion

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

Explanation of terminology

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

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

Substance classes are units of the organisational structure of the *IdentModule*. The substance classes are substance [databases](#) which are also broadly independently subscribable. On the one hand, the liquid and semi-solid substances are separated from the solid powders because they are measured against different references and therefore the spectra cannot be compared. On the other hand, for example the Pharmacopoeia substances are kept separated from the manufacturer-specific databases for TCM (traditional Chinese medicine) raw materials.

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, *Huang Qi* granulate from the company *HerbaSinica* neither needs to be delimited from *Huang Qi* granulate from the company *PhytoComm* nor is matching required. Respectively one single [chemometric model](#) is behind a substance class. (Even if several reciprocally secured chemometric models would be permissible.) The terms *substance class*, *chemometric model* and *databases* are mostly used here as synonyms.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The false positive result describes a spectrum falsely classified as non-identity during validation. This is the most critical type of possible false classification. It means that a substance *A* within identity checking as substance *B* is judged as “*identified*”. For successful validation of an *IdentModule*, a number of false positive events of zero are demanded for all spectra entering the validation. The exception to this restriction is the class of TCM granulates from the company *PhytoComm* as described under [Particularities of individual substance classes](#).

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

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

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

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

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

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

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

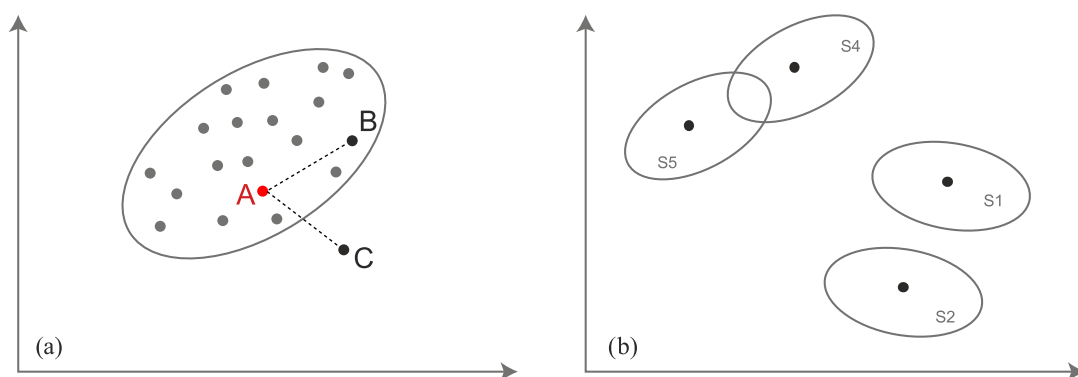


Figure 1: (a) The *Mahalanobis distance* from *A* to *B* is less than from *A* to *C*. However, the Euclidean distances are identical. (b) The *Mahalanobis distance* between the two measurement series *S4* and *S5* is smaller than between *S1* and *S2*. However, the Euclidean distances are identical.

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

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

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

As sample applies the substance from a package. Multiple extractions of substance from the same package for spectrum recordings will be ascribed to the same sample. This also applies if multiple of such samples originate from the same batch.

Does a supplier conversely take 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 156 379 spectra from 21 987 different batches for a total of 448 substances were used to validate the substance class *APIs & excipients, liquid/semi-solid (with analysis certificate)*.

Validation samples

The validation samples can be categorised as follows:

Type A Calibration spectra. These are the spectra used to generate the chemometric model. They were recorded 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 (with analysis certificate)	225	798	34 344

From category *A* a total of 34 344 spectra from 798 batches for a total of 225 substances were taken into account for validation.

Type 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 (with analysis certificate)	440	1501	63 594

From category *B* a total of 63 594 spectra from 1501 batches for a total of 440 substances were taken into account for validation.

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

Substance class	Substances	Batches	Spectra
APIs & excipients, liquid/semi-solid (with analysis certificate)	329	20 595	58 441

From category *C* a total of 58 441 spectra from 20 595 batches for a total of 329 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 (with analysis certificate)* 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 (with analysis certificate)* 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	34 344	0	5 014 224
Type B	0	48 580	1279	9 295 220
Type C	0	51 243	2580	8 535 261

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

	Specificity	Recognition rate
Type A	100.000 00 % (> 99.999 79 %)	100.000 00 % (> 99.969 05 %)
Type B	100.000 00 % (> 99.999 80 %)	94.870 85 % (> 94.844 03 %)
Type C	100.000 00 % (> 99.997 26 %)	91.938 02 % (> 91.701 15 %)

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

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

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

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Acetic acid 30%**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30487-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Acetic acid 30%; Acidum aceticum 30 %; Acidum aceticum dilut. 30%

Special notes

When selecting the *Acetic acid 30%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Acetic acid 30%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acetic acid 30%	11271701	30487	40	1402586
Caelo	Acetic acid 30%	12376101	31131	40	20130107
Caelo	Acetic acid 30%	12376101	31318	40	20130107

Validation samples

A total of 156 379 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 *Acetic acid 30%*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Acetic acid 30%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acetic acid 30%	82207428	30258	40
Caelo	Acetic acid 30%	12376101	31318 [†]	20

- 63 534 spectra from a total of 1475 batches from further 439 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 33 *Apo-Ident* customers from 9 batches from the substance/substance group *Acetic acid 30%*.

Supplier	Substance	Batch	Spectra
Caelo	Acetic acid 30%	14208501	10
Caelo	Acetic acid 30%	16079301	4
Caelo	Acetic acid 30%	12376101	12

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Spectra
GEHE am 21.05.2014	Acetic acid 30%	12376101	1
Caesar & Loretz GmbH	Acetic acid 30%	14208501	1
Caelo	Acetic acid 30%	14058001	1
Caelo	Acetic acid 30%	11271702	2
Caelo	Acetic acid 30%	10313102	1
Kehr	Acetic acid 30%	11271701	1
Caelo	Acetic acid 30%	12376102	1
Caelo	Acetic acid 30%	11271701	3
Phoenix	Acetic acid 30%	11271702	1
Phönix	Acetic acid 30%		1

- 58 402 spectra from 332 *Apo-Ident* customers from a total of 20 084 batches from a further 328 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 *Acetic acid 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 *Acetic acid 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	120	0	34 224
Type B	0	50	10	63 534
Type C	0	36	3	58 402

The substance/substance group *Acetic acid 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	83.3333 % (> 78.3333 %)
Type C	100.0000 % (> 99.5965 %)	92.3077 % (> 84.6154 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30487	30487	0.00	47.86
31131	30487	5.81	46.87
31318	30487	16.13	44.35

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Acetic acid 99%**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30486-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Acetic acid 99%; Acidum aceticum glaciale

Special notes

When selecting the *Acetic acid 99%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Acetic acid 99%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acetic acid 99%	11186701	30486	70	1401607
Caelo	Acetic acid 99%	13013101	31132	39	20130114
Caelo	Acetic acid 99%	13013101	31319	40	20130114

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 149 spectra of 3 reference samples from the substance/substance group *Acetic acid 99%*. These samples are listed above in the [calibration samples](#) section.
- 34 195 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 30 spectra of 2 reference samples from the substance/substance group *Acetic acid 99%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acetic acid 99%	11186701	30486 [†]	10
Caelo	Acetic acid 99%	13013101	31319 [†]	20

- 63 564 spectra from a total of 1475 batches from further 439 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.

- 56 spectra from 47 *Apo-Ident* customers from 19 batches from the substance/substance group *Acetic acid 99%*.

Supplier	Substance	Batch	Spectra
Caelo	Acetic acid 99%	13218301	11
Devisa/Noweda	Acetic acid 99%	13218301	1
Caelo	Acetic acid 99%	13218501	1

continued on the next page

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

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Supplier	Substance	Batch	Spectra
Caelo	Acetic acid 99%	10135706	1
Caelo	Acetic acid 99%	11349901	5
Caelo	Acetic acid 99%	16238401	1
Sanacorp	Acetic acid 99%	11349901	1
Caelo	Acetic acid 99%	13218401	1
Hedinger	Acetic acid 99%	223018B	1
Caelo	Acetic acid 99%	13013101	5
Sanacorp	Acetic acid 99%	13218301	1
Hedinger/NOWEDA	Acetic acid 99%	223012B	1
Hedinger/Jenne	Acetic acid 99%	223044B	1
Caelo	Acetic acid 99%	15280701	3
Hedinger	Acetic acid 99%	223052B	1
Fischar/Gehe	Acetic acid 99%	7003053	1
Otto Fischar GmbH	Acetic acid 99%	7003053	1
Fischar	Acetic acid 99%	7003053	1
Fischar/Phönix	Acetic acid 99%	7004111	1
Otto Fischar / Phoenix	Acetic acid 99%	7003053	1
Phoenix	Acetic acid 99%	7003053	1
otto fischar	Acetic acid 99%	7004111	1
Hedinger	Acetic acid 99%	5113M-01010	1
otto-fischar/gehe	Acetic acid 99%	7004051	2
Fischer/Phönix	Acetic acid 99%	7004111	1
Hedinger/AHD	Acetic acid 99%	2230128	1
Fischar/Gehe	Acetic acid 99%	7002031	1
Fischar/Phoenix	Acetic acid 99%	7002031	1
Otto Fischer GmbH	Acetic acid 99%	7002031	1
Otto Fischar / Phoenix	Acetic acid 99%	7002101	1
ph.eur /phönix	Acetic acid 99%	7002101	1
Anzag	Acetic acid 99%	7002101	1
Fagron	Acetic acid 99%	7002101	1
Fischar/Phoenix	Acetic acid 99%	7002101	1
Fischar / Anzag	Acetic acid 99%	7002031	1

- 58 385 spectra from 332 *Apo-Ident* customers from a total of 20 073 batches from a further 328 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 *Acetic acid 99%* 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 *Acetic acid 99%* 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	149	0	34 195
Type B	0	30	0	63 564
Type C	0	56	0	58 385

The substance/substance group *Acetic acid 99%* 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 % (> 99.9690 %)	100.0000 % (> 95.9732 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 80.0000 %)
Type C	100.0000 % (> 99.5964 %)	100.0000 % (> 89.2857 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30486	30486	0.00	90.24
31132	30486	10.10	93.33
31319	30486	9.37	86.50

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Acetone**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30539-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Acetone; Acetinum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Acetone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Hedinger	Acetone	011215B	31575	40	1505477
Otto Fischar	Acetone	4203051	31580	40	20130513
Hedinger	Acetone	011242B	31793	40	20150703
Otto Fischar	Acetone	4205031	31796	40	20150305

Validation samples

A total of 156 379 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 *Acetone*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 199 spectra of 7 reference samples from the substance/substance group *Acetone*.

Supplier	Substance	Batch	Sample ID	Spectra
Hedinger	Acetone	11152B	30539	40
Otto Fischar	Acetone	pending	30564	40
Hedinger	Acetone	11215B	31575 [†]	19
Otto Fischar	Acetone	4203051	31580 [†]	20
Hedinger	Acetone	11242B	31793 [†]	20
Otto Fischar	Acetone	4205031	31796 [†]	20
Hedinger	Acetone	11236B	32920	40

- 63 395 spectra from a total of 1471 batches from further 439 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.

- 344 spectra from 120 *Apo-Ident* customers from 136 batches from the substance/substance group *Acetone*.

[†]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*.

Supplier	Substance	Batch	Spectra
Hedinger	Acetone	11143B	3
Hedinger	Acetone	11065B	1
Hedinger	Acetone	11134B	1
Hedinger	Acetone	11139b	1
Hedinger	Acetone	11139B	1
Hedinger, Heiligenwiese...	Acetone	11148B	1
Hedinger	Acetone	11148B	3
Hedinger	Acetone	111588	1
Caelo	Acetone	11152b	1
Phönix/ Hedinger	Acetone	11158B	1
Hedinger	Acetone	11152B	1
Hedinger/Noweda	Acetone	111528	1
Anzag/Dr. Seeger	Acetone	111488	1
Hedinger Jenne	Acetone	11158B	1
Anzag/ Hedinger	Acetone	11158B	1
Hedinger	Acetone	11158B	3
Großhandel	Acetone	11158B	1
Hedinger/Gehe	Acetone	11158B	1
Hedinger/AHD	Acetone	11158B	1
Hedinger, Noweda	Acetone	11163B	1
Hedinger	Acetone	11163B	3
Hedinger	Acetone	11168B	1
Hedinger , Noweda	Acetone	11168B	1
Hedinger	Acetone	111688	1
Großhandel	Acetone	11168B	1
Hedinger/Otto	Acetone	111738	1
Caelo	Acetone	111738	1
Hedinger/Phönix	Acetone	11168B	1
Hedinger	Acetone	11173B	11
Hedinger / Gehe	Acetone	11173B	1
Hedinger	Acetone	111738	1
Hedinger/Anzag	Acetone	11173B	1
Anzag	Acetone	11173B	1
Herdinger Phönix	Acetone	11173B	1
Apoth.E.Bartel / Noweda	Acetone	11173B	1
Hedinger/ Noweda	Acetone	11177B	1
Hedinger	Acetone	111828	1
Hedinger	Acetone	11182B	2
Gehe 06.05.2013	Acetone	111828	1
Hedinger/Gehe	Acetone	11177B	1
Barthel	Acetone	11177B	1
Hedinger/Noweda	Acetone	111858	1
Hedinger , Stuttgart	Acetone	11182B	1
Hedinger	Acetone	11177B	1
Hedinger/Anzag	Acetone	11182B	1
heddinge	Acetone	11185B	2
Anzag/Seeger	Acetone	11185B	1
Caelo	Acetone	11185B	2
Hedinger/Phoenix	Acetone	11185B	1
Hedinger/Sanacorp	Acetone	11185B	1
Hedinger/Anzag 03.06.2013	Acetone	11185B	1
Hedinger/Sanacorp	Acetone	11187B	2
Hedinger/ Noweda	Acetone	11187B	1
Hedinger	Acetone	11188B	4
Hedinger	Acetone	111888	1
Hedinger	Acetone	11187B	1
Hedinger/Noweda	Acetone	111888	1
Hedinger / Sanacorp	Acetone	11188B	1
Dr.Seeger GmbH.	Acetone	11188B	1
Hedinger, Noweda	Acetone	11188B	1

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Supplier	Substance	Batch	Spectra
Hedinger	Acetone	111938	1
Hedinger/Otto	Acetone	11193B	1
Hedinger	Acetone	11193B	1
Hedinger/Phönix	Acetone	11195B	1
Euro OTC	Acetone	11193B	1
Hedinger	Acetone	11195B	2
PHOENIX	Acetone	11195B	2
Hedinger	Acetone	11199B	4
Seege/ Jenne	Acetone	11199B	2
Hedinger	Acetone	11200B	1
Hedinger/V.d.L.	Acetone	11199B	1
Hedinger/ Jenne	Acetone	11200B	1
Hedinger/Sanacorp	Acetone	11200B	1
Dr.Seeger GmbH	Acetone	11199B	1
Hedinger / Sanacorp	Acetone	112038	1
Hed	Acetone	11203B	2
Hedinger Phönix	Acetone	112008	1
Hedinger / Noweda	Acetone	11199B	1
hedinger	Acetone	11210B	4
Alliance Health 04.06.2...	Acetone	11199B	1
Hedinger/Noweda	Acetone	11210B	1
Hedinger	Acetone	11210B	5
Hedinger	Acetone	112108	1
Hedinger/Gehe	Acetone	11210B	1
Stumpf/Hedinger	Acetone	11210B	1
Hedinger / Sanacorp	Acetone	11210B	1
Hedinger/Sanacorp	Acetone	11210B	1
Hedinger	Acetone	11210B	1
Apoth.E. Bartel	Acetone	11210B	1
AHD/18.11.14/Hedinger	Acetone	112158	1
Hedinger / Noweda	Acetone	112158	1
Sanacorp/Phoenix	Acetone	11210B	1
Hedinger/Phoenix	Acetone	11215B	1
Hedinger	Acetone	11215B	3
Caelo	Acetone	11218B	1
Phönix	Acetone	11215b	1
Caelo	Acetone	11224B	1
Noweda	Acetone	11224B	1
Hedinger/Phoenix	Acetone	11224B	2
Alliance health 12.01.15	Acetone	11218B	1
Noweda	Acetone	11226B	1
Hedinger/Noweda	Acetone	11224B	1
Hedinger/Noweda	Acetone	11226B	2
Hedinger/Kehr	Acetone	11227B	1
Hedinger	Acetone	11226B	1
Hedinger/Gehe	Acetone	11227B	1
Hedinger/Noweda	Acetone	11232B	1
Caelo	Acetone	11227B	1
Infectopharm	Acetone	11227B	1
Hedinger/Sanacorp	Acetone	11234B	1
Hedinger	Acetone	11232B	3
Phoenix	Acetone	11234B	2
Phönix	Acetone	11234B	1
Hedinger/Phoenix	Acetone	11232B	1
Hedinger	Acetone	11234B	1
Hedinger/Noweda	Acetone	11234B	1
Caelo	Acetone	11247B	1
Hedinger über Phoenix	Acetone	11247B	1
Hedinger / Noweda	Acetone	11236B	2
Hedinger	Acetone	11250B	2

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Supplier	Substance	Batch	Spectra
Hedinger/Phönix	Acetone	11250B	1
Hedinger	Acetone	11241b	1
Noweda/Hedinger	Acetone	11252B	1
Hedinger	Acetone	11256B	1
Hedinger	Acetone	11260B	2
Caelo	Acetone	11252B	1
Hedinger/Phönix	Acetone	11260B	1
Hedinger/Phoenix	Acetone	11260B	1
Caelo	Acetone	11271B	2
Hedinger	Acetone	11272B	2
Hedinger/Noweda	Acetone	11263B	1
Fischar	Acetone	4091513	1
Fischbar	Acetone	4101302	1
Fischbar	Acetone	2101205	1
Fischar	Acetone	2051408	1
Fischar	Acetone	2051409	1
Hedinger	Acetone	4061306	1
Hedinger	Acetone	10091304	1
Otto Fischar	Acetone	1016031	1
Fischar	Acetone	6021303	1
Hedinger/AHD	Acetone	110958A2010	1
Fischar	Acetone	5041403	1
Otto Fischar GmbH & Co...	Acetone	1015041	1
Hedinger	Acetone	8121401	1
otto fischar	Acetone	12011501	1
Hedinger/ Phoenix	Acetone	1214M1002	1
Hiperscan	Acetone		1
otto fischar	Acetone	14031502	1
Fischar	Acetone	16101206	1
Fischar	Acetone	123456	1
Hedinger	Acetone	16061404	1
Hedinger	Acetone	18011306	1
Hedinger	Acetone	16081301	1
Fischbar	Acetone	17091206	1
Hedinger	Acetone	16101402	1
Hedinger	Acetone	19041301	1
Hedinger	Acetone	220114	1
Fischar	Acetone	22111302	1
Hedinger	Acetone	2704211002	1
Fischbar	Acetone	22091201	1
Hedinger	Acetone	25071411	1
Hedinger	Acetone	2713M1002	1
otto fischar	Acetone	23061503	1
Fischar	Acetone	25101302	1
Fischar	Acetone	30081301	1
Fischer/Gehe	Acetone	4201051	1
Hedinger/Gehe	Acetone	311092	1
Kehr	Acetone	4202021	1
Phönix/Fischer	Acetone	4202052	1
Fischar/ Phönix	Acetone	4202022	1
Phönix/Fischar	Acetone	4202052	2
fischer/Anzag	Acetone	4202061	1
Fischar	Acetone	28031301	1
Fischar	Acetone	4008978161101	1
Fischar	Acetone	4202061	1
Phönix/Fischar	Acetone	4202061	3
Phönix/Fischar	Acetone	4202062	1
Fischar/ Phönix	Acetone	4202101	2
Fischar/Gehe	Acetone	4202101	1
Otto Fischar/Phoenix	Acetone	4202112	1

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Supplier	Substance	Batch	Spectra
Fischar	Acetone	4202101	1
Phönix	Acetone	4202112	1
Fischar	Acetone	4203011	4
Fischer/Sanacorp	Acetone	420301	1
Fischar	Acetone	4202121	1
Fischar/ Phönix	Acetone	4203031	27
Fischar/Gehe	Acetone	4203031	3
otto fischar, gehe	Acetone	4203032	2
Fischar	Acetone	4203051	10
Fischar	Acetone	4203032	1
Otto Fischer/ Gehe	Acetone	4203101	1
Fischar/ Now	Acetone	4203111	1
Fischar/Gehe	Acetone	4203101	1
Fischar/Phönix	Acetone	4204012	2
Otto Fischar	Acetone	4203101	1
Fischar/Noweda	Acetone	4203101	1
Sanacorp/ Fischar	Acetone	4203111	1
Fischar	Acetone	4203091	1
otto fischar/gehe	Acetone	4204032	1
Fischar	Acetone	4204031	2
Otto Fischar GmbH&Co.KG...	Acetone	4204032	1
Fischar	Acetone	4204052	1
Otto Fischbar	Acetone	4204052	1
Anzag/ Otto Fischar GmbH...	Acetone	4204032	1
Euro OTC	Acetone	4204032	1
Phönix Gotha	Acetone	4204032	1
Fischar	Acetone	4204071	1
Fischar/Gehe	Acetone	4204071	1
Otto Fischar/Phönix	Acetone	4205012	1
Fischar	Acetone	4205011	1
Fischar	Acetone	4205061	1
Fischar	Acetone	4204072	1
Fischar/Gehe	Acetone	4205071	1
Otto Fischar GmbH / Gehe	Acetone	4205092	1
Otto Fischer/ Gehe	Acetone	4204091	1
Fischer/Gehe 3.11.15	Acetone	4205062	1
Fischar/Alliance Heathc...	Acetone	4206011	1
Caesar & Loretz GmbH Hi...	Acetone	420511	2
Fischar/Gehe	Acetone	4205092	1
Fischar	Acetone	4206041	1
Otto Fischar GmbH & Co...	Acetone	4206012	1
Caesar & Loretz GmbH Hi...	Acetone	4205111	1
Ebert KKH 29.09.2016	Acetone	4206042	1
Caelo	Acetone	59/AKD1	1
Otto Fischar / Noweda	Acetone	4206012	1
Caelo	Acetone		1
Sanacorp	Acetone		2
Noweda	Acetone	901101	1
Otto Fischar	Acetone	90110/1	1
Otto Fischar	Acetone	9011/01	1
Fischar/Phönix	Acetone	4206041	1
Fischer	Acetone	A-040613-3	1
Otto Fischar	Acetone	90205/1	1
Fischar	Acetone	90110/1	1
Hedinger/Phönix	Acetone	11173B	2
Hedinger/AHD	Acetone	11227B	1
Hedinger Jenne	Acetone	11193B	1
Hedinger/Phoenix	Acetone	11187B	1
Hedinger/ Anzag	Acetone	111588	1
GEHE	Acetone	4202052	1

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Supplier	Substance	Batch	Spectra
Holdermann	Acetone	11158B	1
Fishar	Acetone	4202062	1
Caelo	Acetone	606001008	1

- 58 097 spectra from 332 *Apo-Ident* customers from a total of 19 958 batches from a further 328 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 *Acetone* 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 *Acetone* 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	34 184
Type B	0	199	0	63 395
Type C	0	312	32	58 097

The substance/substance group *Acetone* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 96.9849 %)
Type C	100.0000 % (> 99.5963 %)	90.6977 % (> 89.8256 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31575	31575	0.00	142.02
31580	31575	5.43	138.59
31793	31575	3.18	140.81
31796	31575	6.30	135.93

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Acorus oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31159-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Acorus oil; Oleum calami rectific.

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Acorus oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acorus oil	12356706	31159	40	1404623
Caelo	Acorus oil	15081901	32180	40	20150320
Caelo	Acorus oil	15081901	32348	40	20150320

Validation samples

A total of 156 379 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 *Acorus oil*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 1 reference samples from the substance/substance group *Acorus oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acorus oil	15081902	32347	40

- 63 554 spectra from a total of 1476 batches from further 439 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 *Acorus oil*.
- 58 441 spectra from 332 *Apo-Ident* customers from a total of 20 092 batches from a further 329 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 *Acorus 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 *Acorus 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	34 224
Type B	0	40	0	63 554
Type C	0	0	0	58 441

The substance/substance group *Acorus 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31159	31159	0.00	34.32
32180	31159	4.87	31.33
32348	31159	5.32	29.78

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	All-rac-alpha-tocopheryl acetate
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31020-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

All-rac-alpha-tocopheryl acetate; int-rac-alpha-Tocopherylis acetate; Tocopherylis acetatis

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *All-rac-alpha-tocopheryl acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	All-rac-alpha-to...	12362307	31020	40	1402688
Caelo	All-rac-alpha-to...	13396304	31371	40	20131211
Euro OTC	All-rac-alpha-to...	1411025-01	31646	40	20141216
Euro OTC	All-rac-alpha-to...	1512007	31817	40	20151216*

Validation samples

A total of 156 379 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 *All-rac-alpha-tocopheryl acetate*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 228 spectra of 7 reference samples from the substance/substance group *All-rac-alpha-tocopheryl acetate*.

Supplier	Substance	Batch	Sample ID	Spectra
zu erfassen	All-rac-alpha-tocopheryl ace...	pending	30299	30
Caelo	All-rac-alpha-tocopheryl ace...	10159809	30323	40
Euro OTC	All-rac-alpha-tocopheryl ace...	1201009-01	30512	40
Euro OTC	All-rac-alpha-tocopheryl ace...	1411025-01	31646 [†]	18
Euro OTC	All-rac-alpha-tocopheryl ace...	1512007	31817 [†]	20
Euro OTC	All-rac-alpha-tocopheryl ace...	1604060	32286	40
Euro OTC	All-rac-alpha-tocopheryl ace...	1606011	32469	40

- 63 366 spectra from a total of 1471 batches from further 439 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.

*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.

[†]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*.

- 280 spectra from 104 *Apo-Ident* customers from 98 batches from the substance/substance group *All-rac-alpha-tocopheryl acetate*.

Supplier	Substance	Batch	Spectra
Euro OTC	All-rac-alpha-tocopheryl ace...	1310005-01	1
Caelo	All-rac-alpha-tocopheryl ace...	13075202	2
Caelo	All-rac-alpha-tocopheryl ace...	13201102	1
Caelo	All-rac-alpha-tocopheryl ace...	13217201	12
Caelo	All-rac-alpha-tocopheryl ace...	13217205	8
Caelo	All-rac-alpha-tocopheryl ace...	13217202	3
Caelo	All-rac-alpha-tocopheryl ace...	13217207	6
Caesar & Loretz	All-rac-alpha-tocopheryl ace...	13217205	1
Caelo	All-rac-alpha-tocopheryl ace...	13396305	2
Alliance health 05.01.15	All-rac-alpha-tocopheryl ace...	13396305	1
Caelo	All-rac-alpha-tocopheryl ace...	13396306	3
Euro OTC	All-rac-alpha-tocopheryl ace...	1405032-01	2
Caelo	All-rac-alpha-tocopheryl ace...	14076806	5
Caelo	All-rac-alpha-tocopheryl ace...	14076805	8
Caelo	All-rac-alpha-tocopheryl ace...	14011512	1
Euro OTC	All-rac-alpha-tocopheryl ace...	140503201	1
Caelo	All-rac-alpha-tocopheryl ace...	14076808	1
Caelo	All-rac-alpha-tocopheryl ace...	14076812	4
Caelo	All-rac-alpha-tocopheryl ace...	14076813	2
Euro OTC	All-rac-alpha-tocopheryl ace...	1411025-01	4
Caelo	All-rac-alpha-tocopheryl ace...	14363405	4
Caelo	All-rac-alpha-tocopheryl ace...	14363406	5
Noweda 06.04.2016	All-rac-alpha-tocopheryl ace...	14363406	1
Caelo	All-rac-alpha-tocopheryl ace...	14363402	2
Caelo	All-rac-alpha-tocopheryl ace...	14363407	3
Noweda	All-rac-alpha-tocopheryl ace...	14363410	1
Caelo	All-rac-alpha-tocopheryl ace...	14363408	2
Caelo	All-rac-alpha-tocopheryl ace...	1504020-01	4
Euro OTC	All-rac-alpha-tocopheryl ace...	1504020	1
Euro OTC	All-rac-alpha-tocopheryl ace...	1504020-01	2
Caelo	All-rac-alpha-tocopheryl ace...	14363410	4
Caelo	All-rac-alpha-tocopheryl ace...	15126801	2
Euro OTC	All-rac-alpha-tocopheryl ace...	1512007-01	1
Caelo	All-rac-alpha-tocopheryl ace...	15239001	1
Caelo	All-rac-alpha-tocopheryl ace...	15239002	1
Euro OTC	All-rac-alpha-tocopheryl ace...	1504020-02	1
Caelo	All-rac-alpha-tocopheryl ace...	15239003	7
Noweda	All-rac-alpha-tocopheryl ace...	15239011	1
Caelo	All-rac-alpha-tocopheryl ace...	15239012	1
Audor Pharma	All-rac-alpha-tocopheryl ace...	AP13396303T	4
Audor Pharma	All-rac-alpha-tocopheryl ace...	AP143634003	1
Fagron	All-rac-alpha-tocopheryl ace...	225800-0001	1
Euro OTC	All-rac-alpha-tocopheryl ace...	303462	1
DSM Nutritional Prod./...	All-rac-alpha-tocopheryl ace...	15E18-B07	1
Audor Pharma	All-rac-alpha-tocopheryl ace...	AP14363403T	5
Caelo	All-rac-alpha-tocopheryl ace...	26011601	1
Caelo	All-rac-alpha-tocopheryl ace...	15239010	1
Audor Pharma	All-rac-alpha-tocopheryl ace...	AP11300004	1
Audor Pharma	All-rac-alpha-tocopheryl ace...	AP12362305T	5
Audor Pharma	All-rac-alpha-tocopheryl ace...	AP13396303	1
Caelo	All-rac-alpha-tocopheryl ace...	611toc	1
Caelo	All-rac-alpha-tocopheryl ace...	12053809	1
Caelo	All-rac-alpha-tocopheryl ace...	12319401	2
Caelo	All-rac-alpha-tocopheryl ace...	70913Toc	1
Wepa	All-rac-alpha-tocopheryl ace...	AP15239006T	1
Caelo	All-rac-alpha-tocopheryl ace...	12319402	4
Caelo	All-rac-alpha-tocopheryl ace...	12053802	9

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Supplier	Substance	Batch	Spectra
Caelo	All-rac-alpha-tocopheryl ace...	12362302	14
Caelo	All-rac-alpha-tocopheryl ace...	12362307	16
Sanacorp	All-rac-alpha-tocopheryl ace...	12362307	1
Fagron	All-rac-alpha-tocopheryl ace...	12362307	3
phönix 30.07.2013	All-rac-alpha-tocopheryl ace...	12362307	1
Caelo	All-rac-alpha-tocopheryl ace...	12362404	1
Fagron	All-rac-alpha-tocopheryl ace...	12L14-N06	5
Euro OTC	All-rac-alpha-tocopheryl ace...	1301010-01	3
Sanacorp	All-rac-alpha-tocopheryl ace...	1301010-01	1
Großhandel	All-rac-alpha-tocopheryl ace...	13217201	1
Caelo	All-rac-alpha-tocopheryl ace...	1321702	1
Audor Pharma	All-rac-alpha-tocopheryl ace...	AP12362305	1
Caelo	All-rac-alpha-tocopheryl ace...	16091301	1
Euro OTC	All-rac-alpha-tocopheryl ace...	1411025	1
Caelo	All-rac-alpha-tocopheryl ace...	19071302	1
Audor Pharma	All-rac-alpha-tocopheryl ace...	AP11300004T	5
Caesar & Loretz GmbH Hi...	All-rac-alpha-tocopheryl ace...	11300004	1
Fagron	All-rac-alpha-tocopheryl ace...	14G02-B05-3043462	1
Caesar & Loretz GmbH	All-rac-alpha-tocopheryl ace...	15239011	1
Fagron	All-rac-alpha-tocopheryl ace...	14B03-B06-294690	1
Caelo	All-rac-alpha-tocopheryl ace...	15239011	1
Caelo	All-rac-alpha-tocopheryl ace...	12053803	4
Fagron	All-rac-alpha-tocopheryl ace...	12I28-B40	2
Noweda	All-rac-alpha-tocopheryl ace...	912303112	1
Caelo	All-rac-alpha-tocopheryl ace...	3312M-02500	1
Sanacorp	All-rac-alpha-tocopheryl ace...	Ap12362305T	1
Caelo	All-rac-alpha-tocopheryl ace...	1813M-02500	1
Fagron	All-rac-alpha-tocopheryl ace...	UT12020065	1
Caelo	All-rac-alpha-tocopheryl ace...	1411025	1
Fagron	All-rac-alpha-tocopheryl ace...	15e18-b07-311818	1
Fagron	All-rac-alpha-tocopheryl ace...	8120	1
Caelo	All-rac-alpha-tocopheryl ace...	10247405	1
Caelo	All-rac-alpha-tocopheryl ace...	11300001	3
Euro OTC	All-rac-alpha-tocopheryl ace...	11300002	1
ANZAG	All-rac-alpha-tocopheryl ace...	12319401	1
Caelo	All-rac-alpha-tocopheryl ace...	11300003	3
Euro OTC	All-rac-alpha-tocopheryl ace...	1208020-01	4
Fagron	All-rac-alpha-tocopheryl ace...	12G12-No7	1
Fagron	All-rac-alpha-tocopheryl ace...	12E16-N06	2
Noweda	All-rac-alpha-tocopheryl ace...	1208020-01	1
Gehe	All-rac-alpha-tocopheryl ace...	UT10100297	1
Audor Pharma	All-rac-alpha-tocopheryl ace...	12362305T	2
Caelo	All-rac-alpha-tocopheryl ace...	14363401	2
Caelo	All-rac-alpha-tocopheryl ace...	11043007	1
Caelo	All-rac-alpha-tocopheryl ace...	11300005	2
EUro/AHD	All-rac-alpha-tocopheryl ace...	1301010-01	1
Sanacorp	All-rac-alpha-tocopheryl ace...	AP11300004T	1
PHOENIX am 27.03.2014	All-rac-alpha-tocopheryl ace...	1310005-01	1
Fagron	All-rac-alpha-tocopheryl ace...	12/28-B40-288705	1
Caelo	All-rac-alpha-tocopheryl ace...	7123623	1
Caelo	All-rac-alpha-tocopheryl ace...	13396304	3
Stumpf / Hedinger	All-rac-alpha-tocopheryl ace...	15126801	1
Caelo	All-rac-alpha-tocopheryl ace...	11043011	1
Caelo	All-rac-alpha-tocopheryl ace...	113000002	1
Caelo	All-rac-alpha-tocopheryl ace...	11300002	3
Anzag ek: 7.71	All-rac-alpha-tocopheryl ace...	11300002	1
Caesar & Loretz GmbH	All-rac-alpha-tocopheryl ace...	12053802	1
Gehe 16.05.2013	All-rac-alpha-tocopheryl ace...	12053809	1
Erika apotheke	All-rac-alpha-tocopheryl ace...	12319402	1
Caelo	All-rac-alpha-tocopheryl ace...	12319042	1

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Supplier	Substance	Batch	Spectra
Caelo	All-rac-alpha-tocopheryl ace...	12319403	1
DSM Nutritional Prod./ ...	All-rac-alpha-tocopheryl ace...	12E16-N06	1
Gehe	All-rac-alpha-tocopheryl ace...	12L14-N06	1
Caelo	All-rac-alpha-tocopheryl ace...	Ch12053802	2
Euro OTC	All-rac-alpha-tocopheryl ace...	1511I-02500	1
Caelo	All-rac-alpha-tocopheryl ace...	Ch11300002	1
Caelo	All-rac-alpha-tocopheryl ace...	20231012-4	1

- 58 161 spectra from 332 *Apo-Ident* customers from a total of 19 994 batches from a further 328 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 *All-rac-alpha-tocopheryl acetate* 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 *All-rac-alpha-tocopheryl acetate* 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	34 184
Type B	0	228	0	63 366
Type C	0	275	5	58 161

The substance/substance group *All-rac-alpha-tocopheryl acetate* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 97.3684 %)
Type C	100.0000 % (> 99.5963 %)	98.2143 % (> 97.1429 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31020	31020	0.00	72.37
31371	31817	2.73	73.22
31646	31020	3.04	72.22
31817	31817	0.00	74.29

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Angelica root oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30939-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Angelica root oil; Angelica archangelica oleum; Oleum angelicae (e radice)

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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
Caelo	Angelica root oil	11352704	30939	50	1403252
Caelo	Angelica root oil	13157610	31632	40	1511618
Caelo	Angelica root oil	163376	33082	40	20161213*

Validation samples

A total of 156379 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 *Angelica root oil*. These samples are listed above in the [calibration samples](#) section.
- 34214 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Angelica root oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Angelica root oil	13157610	31632 [†]	20
Caelo	Angelica root oil	15337207	32929	40

- 63534 spectra from a total of 1475 batches from further 439 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 *Angelica root 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.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Angelica root oil	11352706	1
Caelo	Angelica root oil	15337205	1

- 58 439 spectra from 332 *Apo-Ident* customers from a total of 20 090 batches from a further 328 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	130	0	34 214
Type B	0	60	0	63 534
Type C	0	2	0	58 439

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 % (> 99.9691 %)	100.0000 % (> 95.3846 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.6008 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30939	30939	0.00	27.03
31632	31632	0.00	20.22
33082	33082	0.00	26.53

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Anise oil / Star aniseed oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31158-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Anise oil / Star aniseed oil; Anise oil; Oleum anisi; Oleum anisi stellati; Star anise oil

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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 / Star aniseed oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Star anise oil	13056105	31158	40	1405104
Caelo	Star anise oil	13358202	31404	40	20131105
Euro OTC	Star anise oil	1303017-01	31525	40	20130422
Caelo	Anise oil	14230101	31596	40	AR-15-FG-004287-01

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Anise oil	15148901	31785	40	20150518
Euro OTC	Star anise oil	511026	31810	40	20151214*
Euro OTC	Star anise oil	1609007	32775	40	20160919*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Anise oil / Star aniseed oil*. These samples are listed above in the [calibration samples](#) section.
- 34 064 spectra from a total of 791 batches from further 223 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 190 spectra of 7 reference samples from the substance/substance group *Anise oil / Star aniseed oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Star anise oil	10319003	30205	40
Euro OTC	Star anise oil	1303017-01	31525 [†]	20
Caelo	Anise oil	14230101	31596 [†]	20
Caelo	Anise oil	15148901	31785 [†]	20
Euro OTC	Star anise oil	511026	31810 [†]	20
Caelo	Anise oil	16306802	32930	40
Caelo	Star anise oil	170162	33061	30

- 63 404 spectra from a total of 1470 batches from further 438 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the

*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.

[†]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*.

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.

- 77 spectra from 46 *Apo-Ident* customers from 35 batches from the substance/substance group *Anise oil / Star aniseed oil*.

Supplier	Substance	Batch	Spectra
Caesar & Loretz	Anise oil	14230104	1
Caelo	Anise oil	14230104	1
Caelo	Anise oil	15119401	4
Caelo	Anise oil	15148901	3
Caesar & Loretz	Anise oil	15148904	1
Caelo	Anise oil	15428901	1
Caelo	Star anise oil	12322503	2
Caelo	Star anise oil	14195202	6
Caelo	Star anise oil	13358209	2
Caelo	Star anise oil	145230101	1
Caelo	Star anise oil	12322507	3
Euro OTC	Star anise oil	1303017-01	1
Caelo	Star anise oil	13358208	1
Caelo	Star anise oil	13051404	1
Caelo	Star anise oil	13358202	3
Caelo	Star anise oil	14125501	1
Caelo	Star anise oil	14230104	1
Caelo	Star anise oil	14230102	1
Euro OTC	Star anise oil	1502037-01	2
Caelo	Star anise oil	25082015C	1
Caelo	Star anise oil	29081504	1
Caesar/Noweda	Star anise oil	411I-01953	1
Phönix	Star anise oil	1502037-01	1
Caelo	Star anise oil	27041501	1
Caelo	Star anise oil	5021403	1
Taoasis	Star anise oil	106155	1
Caelo	Star anise oil	15085805	1
Caelo	Star anise oil	11352402	5
Noweda	Star anise oil	11352402	1
Phönix	Star anise oil	11352402	1
Caelo	Star anise oil	11352409	8
Caelo	Star anise oil	1135409	1
Caelo	Star anise oil	1232207	1
Anzag 10.12.12	Star anise oil	1206014-01	1
Caelo	Star anise oil	12322501	2
Klenk	Star anise oil	12322503	1
Gehe 14.06.2013	Star anise oil	12322503	1
Caelo	Star anise oil	12322505	1
Fagron	Star anise oil	12322507	1
Caelo	Star anise oil	13056105	6
Caelo	Star anise oil	21111302	1
Caelo	Star anise oil	13358201	1
Caelo	Star anise oil	28051310	1

- 58 364 spectra from 332 *Apo-Ident* customers from a total of 20 057 batches from a further 327 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 / Star aniseed 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 *Anise oil / Star aniseed oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	34 064
Type B	0	190	0	63 404
Type C	0	76	1	58 364

The substance/substance group *Anise oil / Star aniseed 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 % (> 99.9689 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.5964 %)	98.7013 % (> 94.8052 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31158	31158	0.00	51.89
31404	31810	2.42	54.21
31525	31810	3.97	53.66
31596	31596	0.00	60.75
31785	31596	1.41	58.55
31810	31810	0.00	55.50
32775	32775	0.00	56.02

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Aqueous salicylic acid 50% (non-ionic, hydrophil...**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30520-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Aqueous salicylic acid 50% (non-ionic, hydrophilic cream SR)

Special notes

When selecting the *Aqueous salicylic acid 50% (non-ionic, hydrophilic cream SR)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Aqueous salicylic acid 50% (non-ionic, hydrophilic cream SR)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
apomix	Aqueous salicyli...	21A250913	31119	40	1404661
apomix	Aqueous salicyli...	13B291216	32992	40	20161230

Validation samples

A total of 156 379 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 *Aqueous salicylic acid 50% (non-ionic, hydrophilic cream SR)*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Aqueous salicylic acid 50% (non-ionic, hydrophilic cream SR)*.

Supplier	Substance	Batch	Sample ID	Spectra
apomix	Aqueous salicylic acid 50% (...)	9A130911	30362	20
apomix	Aqueous salicylic acid 50% (...)	4A050412	30520	40

- 63 534 spectra from a total of 1475 batches from further 439 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.

- 64 spectra from 20 *Apo-Ident* customers from 47 batches from the substance/substance group *Aqueous salicylic acid 50% (non-ionic, hydrophilic cream SR)*.

Supplier	Substance	Batch	Spectra
Apomix / Noweda	Aqueous salicylic acid 50% (...)	1B260115	2
Apomix/Alliance Healthc...	Aqueous salicylic acid 50% (...)	2C230215	1
Apomix/Sanacorp	Aqueous salicylic acid 50% (...)	1B260115	1
Apomix	Aqueous salicylic acid 50% (...)	1B260115	1

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Supplier	Substance	Batch	Spectra
PKH GmbH	Aqueous salicylic acid 50% (...)	2C060314	1
PKH Halle/ Phoenix	Aqueous salicylic acid 50% (...)	1C270114	1
Apomix	Aqueous salicylic acid 50% (...)	2C060314	1
Pharmachem/30	Aqueous salicylic acid 50% (...)	38310314	1
Apomix	Aqueous salicylic acid 50% (...)	3B260315	1
Apomix / Sanacorp	Aqueous salicylic acid 50% (...)	3B260315	1
Apomix / Phönix	Aqueous salicylic acid 50% (...)	3C310314	1
Phönix/apomix	Aqueous salicylic acid 50% (...)	4B200514	1
APOMIX / 30	Aqueous salicylic acid 50% (...)	3B310314	1
Noweda/PKH GmbH	Aqueous salicylic acid 50% (...)	4C280415	1
Apomix / Sanacorp	Aqueous salicylic acid 50% (...)	5B270614	1
Apomix / Noweda	Aqueous salicylic acid 50% (...)	6B080715	2
PKH GmbH	Aqueous salicylic acid 50% (...)	6B170714	1
Noweda/apomix	Aqueous salicylic acid 50% (...)	4B280415	1
Apomix / GEHE	Aqueous salicylic acid 50% (...)	6B1708714	1
Apomix / Phönix	Aqueous salicylic acid 50% (...)	6C170714	1
Apomix/Sanacorp	Aqueous salicylic acid 50% (...)	6C170714	1
Apomix/Alliance Healthc...	Aqueous salicylic acid 50% (...)	8B250815	1
Apomix/ Phönix	Aqueous salicylic acid 50% (...)	6C170714	1
Apomix	Aqueous salicylic acid 50% (...)	8C170914	1
Apomix/Noweda	Aqueous salicylic acid 50% (...)	8B250815	1
Apomix / Sanacorp	Aqueous salicylic acid 50% (...)	7B180814	1
PKH Halle/ Noweda	Aqueous salicylic acid 50% (...)	10B011214	1
Apomix	Aqueous salicylic acid 50% (...)	9B051114	1
Apomix/Alliance Healthc...	Aqueous salicylic acid 50% (...)	9C240915	1
Apomix / 11	Aqueous salicylic acid 50% (...)	10B011214	1
Caelo	Aqueous salicylic acid 50% (...)	11B021215	1
Apomix/AHD	Aqueous salicylic acid 50% (...)	10B261015	1
PKH Halle/ Phoenix	Aqueous salicylic acid 50% (...)	22C161013	1
apomix	Aqueous salicylic acid 50% (...)	10C2601015	1
PKH GmbH	Aqueous salicylic acid 50% (...)	25C041213	1
Apomix / Sanacorp	Aqueous salicylic acid 50% (...)	11B021215	1
Apomix/Sanacorp	Aqueous salicylic acid 50% (...)	4B030516	1
Apomix / Noweda	Aqueous salicylic acid 50% (...)	6B140616	2
apomix / Alliance Healt...	Aqueous salicylic acid 50% (...)	3B230316	1
Apomix/Sanacorp	Aqueous salicylic acid 50% (...)	12C211215	1
JENNE	Aqueous salicylic acid 50% (...)	11B041116	1
Apomix / Sanacorp	Aqueous salicylic acid 50% (...)	7B060716	1
Gehe	Aqueous salicylic acid 50% (...)	4A040313	1
Noweda/PKH GmbH	Aqueous salicylic acid 50% (...)	5B250516	1
Phoenix (PKH Halle)	Aqueous salicylic acid 50% (...)	3A110213	1
PhR/Sanacorp	Aqueous salicylic acid 50% (...)	4A05/13	1
Gehe	Aqueous salicylic acid 50% (...)	9A020812	1
Apomix	Aqueous salicylic acid 50% (...)	9A020812	1
apomix	Aqueous salicylic acid 50% (...)	6A030413	1
Phoenix/ PKH Halle	Aqueous salicylic acid 50% (...)	5A030413	1
Gehe	Aqueous salicylic acid 50% (...)	11A300513	1
Apomix / Phönix	Aqueous salicylic acid 50% (...)	12A300513	1
Apomix / Sanacorp	Aqueous salicylic acid 50% (...)	16A250713	1
PKH GmbH	Aqueous salicylic acid 50% (...)	12A300513	1
PKH Halle / Phoenix	Aqueous salicylic acid 50% (...)	21A250913	1
Apomix / Phönix	Aqueous salicylic acid 50% (...)	19A160913	1
Gehe	Aqueous salicylic acid 50% (...)	22B161013	1
Apomix / Phönix	Aqueous salicylic acid 50% (...)	22C161013	1
Klenk	Aqueous salicylic acid 50% (...)	22B161013	1
Apomix / 11	Aqueous salicylic acid 50% (...)	25B041213	1
Apomix	Aqueous salicylic acid 50% (...)	22C161013	1

- 58 377 spectra from 332 *Apo-Ident* customers from a total of 20 045 batches from a further 328 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 *Aqueous salicylic acid 50% (non-ionic, hydrophilic cream 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 *Aqueous salicylic acid 50% (non-ionic, hydrophilic cream 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	80	0	34 264
Type B	0	40	20	63 534
Type C	0	37	27	58 377

The substance/substance group *Aqueous salicylic acid 50% (non-ionic, hydrophilic cream 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	66.6667 % (> 61.6667 %)
Type C	100.0000 % (> 99.5964 %)	57.8125 % (> 53.1250 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31119	31119	0.00	190.45
32992	31119	9.98	194.71

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Banana aroma**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31105-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Banana aroma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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	40	20141202

Validation samples

A total of 156 379 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 *Banana aroma*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 20 spectra of 1 reference samples from the substance/substance group *Banana aroma*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Banana aroma	14353702	31606 [†]	20

- 63 574 spectra from a total of 1476 batches from further 439 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 *Banana aroma*.

Supplier	Substance	Batch	Spectra
Caelo	Banana aroma	12302509	1
Caelo	Banana aroma	14353707	1

[†]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*.

- 58 439 spectra from 332 *Apo-Ident* customers from a total of 20 090 batches from a further 328 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	80	0	34 264
Type B	0	20	0	63 574
Type C	0	2	0	58 439

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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9712 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.6008 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31105	31105	0.00	79.66
31606	31105	3.56	80.59

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Base cream DAC
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30211-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Base cream DAC; Cremor basalis; Unguentum basale

Special notes

When selecting the *Base cream DAC* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Base cream DAC*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Henry Lamotte	Base cream DAC	5215300	30923	80	20120102
Caelo	Base cream DAC	13139901	31043	40	20130513
Euro OTC	Base cream DAC	1304006-01	31252	40	AR-15-FG-014906-01
Caelo	Base cream DAC	14052901	31474	30	AR-15-FG-000163-02
Euro OTC	Base cream DAC	1506025	31709	40	20150618*
Euro OTC	Base cream DAC	1506025	31710	40	20150618*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Base cream DAC	1506026	31711	40	20150618*
Euro OTC	Base cream DAC	1506026	31712	40	20150618*
Euro OTC	Base cream DAC	1506027	31713	40	20150618*
Euro OTC	Base cream DAC	1506027	31714	40	20150618*
Euro OTC	Base cream DAC	1506028	31715	40	20150618*
Euro OTC	Base cream DAC	1506028	31716	40	20150618*
Caelo	Base cream DAC	154204	31964	40	20151218*
Euro OTC	Base cream DAC	39210516	32345	40	20160623

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 590 spectra of 14 reference samples from the substance/substance group *Base cream DAC*. These samples are listed above in the [calibration samples](#) section.
- 33 754 spectra from a total of 788 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 3882 spectra of 93 reference samples from the substance/substance group *Base cream DAC*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Base cream DAC	10096801	30211	11
Henry Lamotte	Base cream DAC	4758200	30254	41
Henry Lamotte	Base cream DAC	5215300	30744	40
Caelo	Base cream DAC	11297201	30891	60
Euro OTC	Base cream DAC	1301023-01	31005	40
Bombastus	Base cream DAC	276100	31059	40
D'Oroderm	Base cream DAC	1346001	31315	40
Caelo	Base cream DAC	14052901	31474 [†]	10
Euro OTC	Base cream DAC	1506025	31709 [†]	20
Euro OTC	Base cream DAC	1506025	31710 [†]	20
Euro OTC	Base cream DAC	1506026	31711 [†]	20

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

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Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Base cream DAC	1506026	31712 [†]	20
Euro OTC	Base cream DAC	1506027	31713 [†]	20
Euro OTC	Base cream DAC	1506027	31714 [†]	20
Euro OTC	Base cream DAC	1506028	31715 [†]	20
Euro OTC	Base cream DAC	1506028	31716 [†]	20
Caelo	Base cream DAC	154198	31963	60
Caelo	Base cream DAC	154204	31964 [†]	20
Caelo	Base cream DAC	154201	31965	60
Caelo	Base cream DAC	153911	31966	60
Caelo	Base cream DAC	153910	31967	60
Caelo	Base cream DAC	153909	31968	60
Caelo	Base cream DAC	153905	31969	60
Caelo	Base cream DAC	153904	31970	60
Caelo	Base cream DAC	153903	31971	60
Caelo	Base cream DAC	153902	31972	60
Caelo	Base cream DAC	153578	31973	60
Caelo	Base cream DAC	153869	31974	60
Caelo	Base cream DAC	153872	31975	60
Caelo	Base cream DAC	153868	31976	60
Caelo	Base cream DAC	153576	31977	60
Caelo	Base cream DAC	160051	31978	60
Caelo	Base cream DAC	160052	31979	60
Caelo	Base cream DAC	160053	31980	60
Caelo	Base cream DAC	160054	31981	60
Caelo	Base cream DAC	160055	31982	60
Caelo	Base cream DAC	161021	32236	40
Caelo	Base cream DAC	161347	32237	40
Caelo	Base cream DAC	161348	32238	40
Caelo	Base cream DAC	161349	32239	40
Caelo	Base cream DAC	161356	32240	40
Caelo	Base cream DAC	161357	32241	40
Caelo	Base cream DAC	161357	32242	40
Caelo	Base cream DAC	161357	32243	40
Caelo	Base cream DAC	161358	32244	40
Caelo	Base cream DAC	161359	32245	40
Caelo	Base cream DAC	161360	32246	40
Caelo	Base cream DAC	161361	32247	40
Caelo	Base cream DAC	161362	32248	40
Caelo	Base cream DAC	161363	32249	40
Caelo	Base cream DAC	161456	32250	40
Caelo	Base cream DAC	161038	32251	40
Caelo	Base cream DAC	160556	32252	40
Caelo	Base cream DAC	160588	32253	40
Caelo	Base cream DAC	160559	32254	40
Caelo	Base cream DAC	161020	32255	40
Caelo	Base cream DAC	161020	32256	40
Caelo	Base cream DAC	161020	32257	40
Caelo	Base cream DAC	161021	32258	40
Caelo	Base cream DAC	161021	32259	40
Caelo	Base cream DAC	161022	32260	40
Caelo	Base cream DAC	161022	32261	40
Caelo	Base cream DAC	161501	32368	40
Caelo	Base cream DAC	161522	32369	40
Caelo	Base cream DAC	161460	32521	40
Caelo	Base cream DAC	162378	32522	40
Caelo	Base cream DAC	161361	32523	40
Caelo	Base cream DAC	161499	32524	40
Caelo	Base cream DAC	161554	32525	40
Caelo	Base cream DAC	162204	32526	40

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Base cream DAC	162205	32527	40
Caelo	Base cream DAC	162379	32528	40
Caelo	Base cream DAC	162380	32529	40
Caelo	Base cream DAC	162381	32530	40
Caelo	Base cream DAC	162382	32531	40
Caelo	Base cream DAC	162383	32532	40
Caelo	Base cream DAC	162403	32533	40
Caelo	Base cream DAC	162406	32534	40
Caelo	Base cream DAC	162407	32535	40
Caelo	Base cream DAC	162407	32536	40
Caelo	Base cream DAC	162407	32537	40
Caelo	Base cream DAC	162407	32538	40
Caelo	Base cream DAC	162410	32539	40
Caelo	Base cream DAC	162416	32540	40
Caelo	Base cream DAC	162417	32541	40
Caelo	Base cream DAC	162420	32542	40
Caelo	Base cream DAC	162422	32543	40
Caelo	Base cream DAC	162617	32544	40
Caelo	Base cream DAC	162617	32545	40
Caelo	Base cream DAC	162617	32546	40
Caelo	Base cream DAC	161500	32547	40
Caelo	Base cream DAC	161524	32548	40
Caelo	Base cream DAC	161558	32549	40

- 59 712 spectra from a total of 1401 batches from further 439 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.

- 3853 spectra from 288 *Apo-Ident* customers from 1452 batches from the substance/substance group *Base cream DAC*.

Supplier	Substance	Batch	Spectra
Noweda	Base cream DAC	13347201	1
Phönix	Base cream DAC	6207	1
Caelo	Base cream DAC	13380901	10
Caelo	Base cream DAC	1319901	3
Caelo	Base cream DAC	14090801	8
Caelo	Base cream DAC	13385301	5
Caelo	Base cream DAC	14092001	5
Caelo	Base cream DAC	14144101	7
Caelo	Base cream DAC	14178001	5
Phoenix Goettin	Base cream DAC	14289601	1
Caelo	Base cream DAC	15040601	6
Caelo	Base cream DAC	15167001	8

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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
Caelo	Base cream DAC	15315401	4
Euro OTC	Base cream DAC	1301022-01	6
Caelo	Base cream DAC	12191901	13
Caelo	Base cream DAC	13173501	4
Noweda	Base cream DAC	131250001	1
Lamotte/AHD	Base cream DAC	589900	1
Bombastus	Base cream DAC	281334	2
Caelo	Base cream DAC	13311401	6
Caelo	Base cream DAC	13139801	5
Caelo	Base cream DAC	13198301	3
Caelo	Base cream DAC	12249501	3
Phönix Gotha	Base cream DAC	5489800	1
HENRYLAMOTTE/Gehe	Base cream DAC	5408000	1
Caelo	Base cream DAC	72/AKD1	1
Lamotte/AHD	Base cream DAC	5489900	5
Gehe	Base cream DAC	276944	1
Gehe	Base cream DAC	278148	3
Ensbona/ Sanacorp	Base cream DAC	1200216	3
Fagron	Base cream DAC	3987	2
Ensbona	Base cream DAC	2020216	1
Caelo	Base cream DAC	2020216	2
Caelo	Base cream DAC	2121403	1
Apomix/Jenne	Base cream DAC	4D061014	1
gehe	Base cream DAC	5A040414	1
Eimermacher	Base cream DAC	8811114	1
Noweda/Ensbona	Base cream DAC	8821114	5
Sanacorp/ Ferd. Eimerma...	Base cream DAC	8821114	2
Ensbona	Base cream DAC	8811114	1
Fagron	Base cream DAC	6879559	1
Caelo	Base cream DAC	1214I01309	1
Eimermacher	Base cream DAC	12170214	2
Euro OTC	Base cream DAC	1301023-01	7
Caelo	Base cream DAC	13051503	1
Gehe	Base cream DAC	1302036-01	1
Caelo	Base cream DAC	1307003-01	1
Euro OTC	Base cream DAC	1307044-01	2
Euro OTC	Base cream DAC	1306030-01	1
Euro OTC	Base cream DAC	1307045-01	1
Phoenix	Base cream DAC	1306002-01	1
Euro OTC	Base cream DAC	1307034-01	3
Euro OTC	Base cream DAC	1307047-01	1
Euro OTC	Base cream DAC	1308022-01	4
Euro OTC	Base cream DAC	1308013-01	3
Euro OTC	Base cream DAC	130704701	2
Caesar & Loretz GmbH Hi...	Base cream DAC	1308013-01	1
Euro OTC	Base cream DAC	13080224-01	1
Euro OTC	Base cream DAC	1308023-01	2
Euro OTC	Base cream DAC	1308024-01	7
Euro OTC	Base cream DAC	1309005-1	2
Euro OTC	Base cream DAC	1309006-01	4
Euro OTC	Base cream DAC	1309007-01	8
Euro OTG	Base cream DAC	1309008-01	2
Euro OTC	Base cream DAC	1309013-01	6
Euro OTC	Base cream DAC	1309008-01	1
Euro OTC	Base cream DAC	1309015-01	3
Euro OTC	Base cream DAC	1311005-01	4
Euro OTC	Base cream DAC	1311004-01	2
Caelo	Base cream DAC	131100701	1
Euro OTC	Base cream DAC	131007-01	1
Euro OTC	Base cream DAC	131100801	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Base cream DAC	131101601	1
Euro OTC	Base cream DAC	1311008-01	1
Caelo	Base cream DAC	1311009-01	1
Euro OTC	Base cream DAC	131103101	1
EuRho/Phoenix	Base cream DAC	1311031-01	1
Euro OTC	Base cream DAC	131200101	1
EuRho/Phönix	Base cream DAC	1312002-01	1
Euro/Gehe	Base cream DAC	1312002-01	1
Euro OTC	Base cream DAC	1312021-01	1
Euro OTC	Base cream DAC	1312035-01	5
Euro OTC	Base cream DAC	1312004-01	1
Euro OTC	Base cream DAC	1312036-01	1
EuRho/Phönix	Base cream DAC	1312037-01	1
Euro OTC	Base cream DAC	1312038-01	1
Euro OTC	Base cream DAC	1312037-01	1
Euro OTC	Base cream DAC	1312039-01	2
Caelo	Base cream DAC	13139901	11
Caelo	Base cream DAC	13158701	1
Caelo	Base cream DAC	13198701	10
Sanacorp	Base cream DAC	13311801	1
Caelo	Base cream DAC	13311801	8
Caelo	Base cream DAC	13249701	5
Caelo	Base cream DAC	13311901	5
Caelo	Base cream DAC	13312001	6
Caelo	Base cream DAC	1334701	1
noweda	Base cream DAC	13347101	1
Caelo	Base cream DAC	13347101	13
Caelo	Base cream DAC	13347201	6
Caelo	Base cream DAC	13347301	7
Caelo	Base cream DAC	13377201	9
Caelo	Base cream DAC	13377901	7
Caelo	Base cream DAC	13378001	10
Caelo	Base cream DAC	13378201	5
Caelo	Base cream DAC	1338091	1
Caelo	Base cream DAC	13381001	12
Caelo	Base cream DAC	13381201	6
Caelo	Base cream DAC	13384901	9
Caelo	Base cream DAC	13381101	1
Caelo	Base cream DAC	13385101	5
Caelo	Base cream DAC	13386001	6
Caelo	Base cream DAC	13385201	2
Caelo	Base cream DAC	13386101	3
Caelo	Base cream DAC	13386201	6
Noweda 17.10.2014	Base cream DAC	1346001	2
Fagron	Base cream DAC	13E22t06003981	1
D'Oroderm	Base cream DAC	1346001	1
Fagron	Base cream DAC	13E21-T09-003910	1
Caelo	Base cream DAC	13E22-T08-003987	1
Fagron	Base cream DAC	13E23-T16-004035	2
Fagron	Base cream DAC	13E23T10004023	1
Fragron	Base cream DAC	13E23-T15-005569	1
Fagron	Base cream DAC	13H14-T01-006203	4
Fagron	Base cream DAC	13H14T01006203	1
Fagron	Base cream DAC	13H14-T04-006218	3
Fagron	Base cream DAC	13H14T080	1
Fagron	Base cream DAC	13H14-T03-006212	1
Fagron	Base cream DAC	13K12-T04008048	1
Fagron	Base cream DAC	13H14-T09	1
Caelo	Base cream DAC	13K12T03008044	1
Fagron	Base cream DAC	13K12-T02-008039	4

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Supplier	Substance	Batch	Spectra
Fagron	Base cream DAC	13K12-T06-008054	2
Fagron	Base cream DAC	13K12-T06-0004	1
Caelo	Base cream DAC	13K12-t07-008057	1
Fagron	Base cream DAC	13K12-T04-008048	1
EuRho	Base cream DAC	13K29-B32-288245	1
Fagron	Base cream DAC	13K12-T08-008063	1
Fagron	Base cream DAC	13K12-T07-008057	1
Euro OTC	Base cream DAC	1401020-01	2
Euro OTC	Base cream DAC	1401022-01	3
Bombastus	Base cream DAC	1401020-01	1
Euro OTC	Base cream DAC	1401023-01	3
Euro OTC	Base cream DAC	1401024-01	4
Euro OTC	Base cream DAC	1401025-01	7
Caelo	Base cream DAC	1401025-01	3
EuRho	Base cream DAC	1401026-01	2
Euro OTC	Base cream DAC	140102601	1
Euro OTC	Base cream DAC	1401026-01	1
Caelo	Base cream DAC	14011515	1
Phönix	Base cream DAC	14035801	1
Caelo	Base cream DAC	14035901	3
Caelo	Base cream DAC	14036101	2
Caelo	Base cream DAC	14036001	2
Caelo	Base cream DAC	14036201	9
Caelo	Base cream DAC	140409	1
Caelo	Base cream DAC	14052901	15
Caelo	Base cream DAC	14053002	1
Caelo	Base cream DAC	14053001	3
Caelo	Base cream DAC	14053401	4
Caelo	Base cream DAC	14053301	2
Caelo	Base cream DAC	14053101	2
Caesar & Loretz	Base cream DAC	14053401	1
Phönix	Base cream DAC	14053501	1
Caelo	Base cream DAC	14053601	3
Caelo	Base cream DAC	14053701	4
Fagron	Base cream DAC	1405-T07-016800	1
GEHE 15.05.2014	Base cream DAC	14053701	1
Euro OTC	Base cream DAC	1407018-01	1
Euro OTC	Base cream DAC	1407021-01	1
Euro OTC	Base cream DAC	1407019-01	1
Euro OTC	Base cream DAC	1407020-01	1
Euro OTC	Base cream DAC	1407054-01	3
Euro OTC	Base cream DAC	1407022-01	1
Euro OTC	Base cream DAC	140702201	1
Caelo	Base cream DAC	140705401	1
Euro OTC	Base cream DAC	140705501	1
Caelo	Base cream DAC	1408009-01	1
Euro OTC	Base cream DAC	1407055-01	2
Caelo	Base cream DAC	14090401	8
Euro OTC	Base cream DAC	1409056-01	1
Sanacorp	Base cream DAC	14090401	1
Caelo	Base cream DAC	1409041	1
Caelo	Base cream DAC	14090601	6
Phoenix 20.06.2014	Base cream DAC	14090601	1
Gehe 28.05.2014	Base cream DAC	14090601	1
Raben-Apotheke Mildenau	Base cream DAC	14090601	1
Caelo	Base cream DAC	14090701	6
Euro OTC	Base cream DAC	14090801	2
Caelo	Base cream DAC	14091401	2
Caelo	Base cream DAC	14091501	8
Caelo	Base cream DAC	14091601	7

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Supplier	Substance	Batch	Spectra
Sanacorp	Base cream DAC	14091501	2
GEHE 24.06.2014	Base cream DAC	14091601	1
Caelo	Base cream DAC	14091701	7
Sanacorp	Base cream DAC	14091701	1
Caelo	Base cream DAC	14091801	5
Caelo	Base cream DAC	14091901	5
Cealo / Noweda	Base cream DAC	14092001	1
Europharm/Otto	Base cream DAC	1411030-01	1
Euro OTC	Base cream DAC	1412002-01	3
ensbona/Noweda	Base cream DAC	14120715	1
Eimermacher/Sanacorp	Base cream DAC	14120715	4
Euro OTC	Base cream DAC	1411031-01	1
Ensbona/Eimermacher	Base cream DAC	14120715	1
Ensbona	Base cream DAC	14130715	1
Ensbona/Eimermacher	Base cream DAC	14130715	1
Caelo	Base cream DAC	14143801	4
Phoenix 13.11.14	Base cream DAC	14143801	1
Caelo	Base cream DAC	14143901	5
Raben-Apotheke Mildenau	Base cream DAC	14143901	1
Caelo	Base cream DAC	14144001	4
Sanacorp	Base cream DAC	14144001	1
Noweda	Base cream DAC	14144101	1
Sanacorp	Base cream DAC	14144101	1
Caelo	Base cream DAC	14144201	3
Caelo	Base cream DAC	14151001	5
Caelo	Base cream DAC	14151301	1
Caelo	Base cream DAC	14151101	2
Caelo	Base cream DAC	14151401	6
Caelo	Base cream DAC	14151501	8
Caelo	Base cream DAC	14151601	5
Caelo	Base cream DAC	14151801	3
Caelo	Base cream DAC	14151901	3
Schmittmann GmbH	Base cream DAC	14151901	1
Caelo	Base cream DAC	14177501	6
Caelo	Base cream DAC	14177701	1
Caelo	Base cream DAC	1417780	1
Caelo	Base cream DAC	14177801	2
Caelo	Base cream DAC	14177901	5
Anzag	Base cream DAC	14177801	1
phoenix 01.10.14	Base cream DAC	14178001	1
Caelo	Base cream DAC	14178101	4
Caelo	Base cream DAC	14178201	10
Caelo	Base cream DAC	14178401	1
Caelo	Base cream DAC	14223201	9
Caelo	Base cream DAC	14222901	1
Euro OTC	Base cream DAC	14223101	1
Caelo	Base cream DAC	14223001	1
Caelo	Base cream DAC	14222801	2
Caelo	Base cream DAC	14227601	2
Caelo	Base cream DAC	14227701	4
Caelo	Base cream DAC	14227801	8
Euro OTC	Base cream DAC	14232001	1
Caelo	Base cream DAC	14228001	1
Sanacorp	Base cream DAC	14227901	1
Caelo	Base cream DAC	14227901	1
Caelo	Base cream DAC	14232001	5
Caelo	Base cream DAC	14232101	3
Caelo	Base cream DAC	14232201	3
Allianz Healthcare 20.0...	Base cream DAC	14232201	1
Caelo	Base cream DAC	14238101	3

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Supplier	Substance	Batch	Spectra
Caelo	Base cream DAC	14238201	1
Caelo	Base cream DAC	14238401	2
Caelo	Base cream DAC	14232301	3
Caelo	Base cream DAC	14238301	2
Caelo	Base cream DAC	14238501	1
Caelo	Base cream DAC	14244501	4
Alliance Healthcare	Base cream DAC	14238501	1
Sanacorp	Base cream DAC	14244501	1
Caelo	Base cream DAC	14263201	1
Caelo	Base cream DAC	14263301	5
Caelo	Base cream DAC	14263601	2
Caelo	Base cream DAC	1426331	1
Caelo	Base cream DAC	14263401	1
Caelo	Base cream DAC	1428201	1
Caelo	Base cream DAC	14289601	3
Caelo	Base cream DAC	14289701	6
Caelo	Base cream DAC	14274601	1
Caelo	Base cream DAC	14289801	10
Sanacorp	Base cream DAC	14289801	1
Caelo	Base cream DAC	14289901	7
Phönix 23.01.15	Base cream DAC	14290001	1
Caelo	Base cream DAC	14290001	3
Caelo	Base cream DAC	142990001	1
Caelo	Base cream DAC	14290101	1
Caelo	Base cream DAC	14303301	1
Caelo	Base cream DAC	14303101	3
Caelo	Base cream DAC	14303801	3
Caelo	Base cream DAC	14303401	1
Caelo	Base cream DAC	14303501	2
Caelo	Base cream DAC	14303901	10
Phönix	Base cream DAC	14303901	1
Caelo	Base cream DAC	14325101	1
Caelo	Base cream DAC	14325401	1
Gehe 25.02.15	Base cream DAC	14325401	1
Dr. Wolff	Base cream DAC	14325601	1
Caelo	Base cream DAC	14326701	4
Caelo	Base cream DAC	14325901	1
Caelo	Base cream DAC	14325801	1
Caelo	Base cream DAC	14325601	2
Caelo	Base cream DAC	14325701	1
Caelo	Base cream DAC	14326901	3
Sanacorp1	Base cream DAC	14326801	2
Caelo	Base cream DAC	14326801	3
Caelo	Base cream DAC	14327001	4
Caelo	Base cream DAC	14327101	2
Caelo	Base cream DAC	14327301	2
Caelo	Base cream DAC	14327501	2
Caelo	Base cream DAC	14327401	2
Caelo	Base cream DAC	14327601	3
Sanacorp	Base cream DAC	14327501	1
Caelo	Base cream DAC	14327701	3
Caelo	Base cream DAC	14327801	2
Caelo	Base cream DAC	14327901	7
Caelo	Base cream DAC	14328001	1
Caelo	Base cream DAC	14368001	7
Caelo	Base cream DAC	14368201	2
Caelo	Base cream DAC	14368101	1
Caelo	Base cream DAC	14374201	3
Caelo	Base cream DAC	14374301	1
Caelo	Base cream DAC	14374401	3

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Supplier	Substance	Batch	Spectra
Caelo	Base cream DAC	14374501	3
Ichthyol / Gehe	Base cream DAC	14A10-T06	1
Fagron	Base cream DAC	14A10-T06-009259	3
Fagron	Base cream DAC	14A10-T06	1
Fagron	Base cream DAC	14A13-T01-009276	1
Fagron	Base cream DAC	14A13-T02-009280	1
Fagron	Base cream DAC	14A13-T04009286	1
Fagron	Base cream DAC	14A13-T05-009289	1
Fagron	Base cream DAC	14B28T04010673	1
Fagron	Base cream DAC	14A13-T07-009298	1
Fagron	Base cream DAC	14D085T045011692	1
Fagron	Base cream DAC	14A13-T06	1
Fagron	Base cream DAC	14d08t02011686	1
Fagron	Base cream DAC	14D08-T01-011683	1
Fagron	Base cream DAC	14D08-T02-011686	1
Phönix	Base cream DAC	14D08-T02-0002	1
Fagron	Base cream DAC	14D08-T03-011689	3
Fagron	Base cream DAC	14D08-T04-011692	5
Fagron	Base cream DAC	14d08-t04-011632	1
Fagron	Base cream DAC	14D08-T05-011697	2
Fagron	Base cream DAC	14D08-T06-011702	1
Fagron	Base cream DAC	14D08-T07-011705	1
Fagron	Base cream DAC	14D08-T08-011710	4
Fagron	Base cream DAC	14F05-T06-012961	4
Fagron	Base cream DAC	14D08-T10-011716	1
Fagron	Base cream DAC	14F05-T07-012965	3
Caelo	Base cream DAC	14f05-t07-012965	1
Fagron	Base cream DAC	14F05-T08-012969	1
Fagron	Base cream DAC	14F05-T24	1
Fagron	Base cream DAC	14F05-T24-012983	7
Fagron	Base cream DAC	14F05-T22-012975	1
Fagron	Base cream DAC	14F06-T04-013010	1
Fagron	Base cream DAC	14F06-T04	1
Gehe,27.0415	Base cream DAC	14F27-T03-013614	1
Fagron	Base cream DAC	14F06-T04-013010	1
Fagron	Base cream DAC	14J06-T08-015886	5
Fagron	Base cream DAC	14I06-T08-015887	1
Fagron	Base cream DAC	14I07-T07-015961	1
Fagron	Base cream DAC	14J07-T06-015957	3
Caelo	Base cream DAC	14j07T06015957	1
Fagron	Base cream DAC	14J07-T07-015961	1
Fagron	Base cream DAC	14J07-T10-015971	1
Fagron	Base cream DAC	14J07-T10-015972	2
Caelo	Base cream DAC	14J07-T11-015975	2
Fagron	Base cream DAC	14J07-T14-015986	1
Fagron	Base cream DAC	14J07-T12	1
Fagron	Base cream DAC	14K05-T06-016796	2
Fagron	Base cream DAC	14K05-T07-016800	3
Fagron	Base cream DAC	14k05t07016800	1
Fagron	Base cream DAC	14K05-T08-016808	1
Sanacorp	Base cream DAC	15000701	1
Fagron	Base cream DAC	14k05-t07016800	1
Caelo	Base cream DAC	15000701	2
Caelo	Base cream DAC	15/138/B	1
Caelo	Base cream DAC	15000801	4
Caelo	Base cream DAC	15000901	5
Caelo	Base cream DAC	15004001	5
Euro OTC	Base cream DAC	1501008-01	3
Euro OTC	Base cream DAC	1501007-01	1
Euro OTC	Base cream DAC	1501009-01	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Base cream DAC	150100801	1
Caelo	Base cream DAC	1501019-01	1
Euro OTC	Base cream DAC	1501020-01	1
Euro OTC	Base cream DAC	1501019-01	1
Caelo	Base cream DAC	1501039-1	1
Euro	Base cream DAC	1501040-01	2
Euro OTC	Base cream DAC	1501050-01	2
Euro OTC	Base cream DAC	1501040-01	1
Euro OTC	Base cream DAC	1501051-01	4
EuRho	Base cream DAC	1501050-01	1
Caelo	Base cream DAC	1501052-01	1
Euro OTC	Base cream DAC	1501052-01	1
Euro OTC	Base cream DAC	1502007-01	1
Euro OTC	Base cream DAC	1501053-01	2
EuRho	Base cream DAC	1502008-01	1
Caelo	Base cream DAC	1502008-01	2
Euro OTC	Base cream DAC	1501055-01	1
Euro OTC	Base cream DAC	1502008-01	3
Euro OTC	Base cream DAC	1502015-01	3
Euro OTC	Base cream DAC	1502016-01	3
Euro OTC	Base cream DAC	1502017-01	5
Euro OTC	Base cream DAC	1502025-01	1
EuRho/Phönix	Base cream DAC	1502017-01	1
EuRho/Noweda	Base cream DAC	1502025-01	1
Phönix Gotha	Base cream DAC	1502025-01	1
Euro OTC	Base cream DAC	1502026-01	2
Caelo	Base cream DAC	1502027-01	1
Euro OTC	Base cream DAC	1502027-01	1
Euro OTC	Base cream DAC	1502028-01	2
EuRho	Base cream DAC	1502029-01	2
Euro OTC	Base cream DAC	1502029-01	1
Caelo	Base cream DAC	15040701	7
Gehe	Base cream DAC	15040801	1
Caelo	Base cream DAC	15041001	4
Caelo	Base cream DAC	15040801	2
Caelo	Base cream DAC	15040901	1
Caelo	Base cream DAC	15041101	6
Euro OTC	Base cream DAC	1506028-01	1
Euro OTC	Base cream DAC	1506045-01	4
Euro OTC	Base cream DAC	1506026-01	1
Euro OTC	Base cream DAC	1506046-01	1
Euro OTC	Base cream DAC	1506053	1
Euro OTC	Base cream DAC	1506047-01	4
Caelo	Base cream DAC	15064301	4
Euro OTC	Base cream DAC	1506053-01	1
Caelo	Base cream DAC	15064401	5
Caelo	Base cream DAC	15064501	3
Caelo	Base cream DAC	15064701	9
Caelo	Base cream DAC	15064601	2
Caelo	Base cream DAC	150671	1
Sanacorp	Base cream DAC	15070101	1
Caelo	Base cream DAC	15070101	7
Euro OTC	Base cream DAC	1507017-01	1
Euro OTC	Base cream DAC	150701701	1
Caelo	Base cream DAC	15070201	8
Caelo	Base cream DAC	15071405	1
Euro OTC	Base cream DAC	1508001-01	9
Caelo	Base cream DAC	15083101	1
Caelo	Base cream DAC	15083001	1
Caelo	Base cream DAC	15083201	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Base cream DAC	1509021-01	6
Euro OTC	Base cream DAC	1509026-01	2
Basiscreme	Base cream DAC	1510027-01	1
Euro OTC	Base cream DAC	1509021-21	1
Euro OTC	Base cream DAC	1510030-01	11
Eurho/Noweda	Base cream DAC	1510030-01	2
Euro OTC	Base cream DAC	1511001-01	5
Euro OTC	Base cream DAC	15110011-01	1
Fagron	Base cream DAC	1511001-01	1
Euro OTC	Base cream DAC	1511002-01	6
Euro OTC	Base cream DAC	1511002-02	1
Euro OTC	Base cream DAC	151100201	1
Euro OTC	Base cream DAC	1512002-01	2
Bombastus	Base cream DAC	1511002-01	1
Caelo	Base cream DAC	15164401	2
Caelo	Base cream DAC	15164301	1
Sanacorp	Base cream DAC	15164601	2
Caelo	Base cream DAC	15164601	3
Caelo	Base cream DAC	15164701	9
Caelo	Base cream DAC	15166601	1
Caelo	Base cream DAC	15166701	1
Caelo	Base cream DAC	15166801	3
Caelo	Base cream DAC	15166901	3
Caelo	Base cream DAC	15173201	4
Caelo	Base cream DAC	15173301	2
Caelo	Base cream DAC	15173401	2
Caelo	Base cream DAC	15173501	5
Caelo	Base cream DAC	15173601	6
Fagron	Base cream DAC	15173601	1
Caelo	Base cream DAC	15184001	2
Caelo	Base cream DAC	15184301	3
Caelo	Base cream DAC	15184401	4
Caelo	Base cream DAC	15184201	1
Caelo	Base cream DAC	15184301	1
Caelo	Base cream DAC	15184101	1
Caelo	Base cream DAC	15190901	2
Caelo	Base cream DAC	15190601	1
Caelo	Base cream DAC	15190701	2
Caelo	Base cream DAC	15191001	4
Caelo	Base cream DAC	15191102	5
Caelo	Base cream DAC	15191201	1
Caelo	Base cream DAC	15191202	5
Caelo	Base cream DAC	15191301	2
Fagron	Base cream DAC	15241801	1
Caelo	Base cream DAC	15241901	3
Caelo	Base cream DAC	15242001	7
Sanacorp	Base cream DAC	15250001	1
Caelo	Base cream DAC	15250001	2
Caelo	Base cream DAC	15250101	4
Caesar&loretz,Anzag	Base cream DAC	15250101	1
Caelo	Base cream DAC	15250201	4
Caelo	Base cream DAC	15250301	4
Caelo	Base cream DAC	15250701	1
Caelo	Base cream DAC	15250601	2
Caelo	Base cream DAC	15250801	3
Caelo	Base cream DAC	15250501	6
Caelo	Base cream DAC	15250902	9
Caelo	Base cream DAC	15272201	11
Caelo	Base cream DAC	15272301	5
Caelo	Base cream DAC	15272402	6

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Supplier	Substance	Batch	Spectra
Caesar&Loretz/Caesar&Lo...	Base cream DAC	15272601	1
Caelo	Base cream DAC	15272601	1
Caelo	Base cream DAC	15306101	1
Caelo	Base cream DAC	15306401	4
Caelo	Base cream DAC	15306501	4
Caelo	Base cream DAC	15306701	2
Sanacorp	Base cream DAC	15315301	1
Calo	Base cream DAC	15306701	1
Caelo	Base cream DAC	15313601	2
Caelo	Base cream DAC	15306601	2
Caelo	Base cream DAC	15315301	3
Caelo	Base cream DAC	15318801	4
Caelo	Base cream DAC	15318901	2
Caelo	Base cream DAC	15357601	12
Caelo	Base cream DAC	15357701	11
Caelo	Base cream DAC	15357801	5
Caelo	Base cream DAC	15386901	4
Bombastus	Base cream DAC	15387001	1
Caelo	Base cream DAC	15387001	3
Caelo	Base cream DAC	15386801	1
Caelo	Base cream DAC	15387101	4
Sanacorp	Base cream DAC	15387101	1
Caelo	Base cream DAC	15387201	2
Caelo	Base cream DAC	15390401	1
Caelo	Base cream DAC	15390501	1
Caelo	Base cream DAC	15390601	2
Caelo	Base cream DAC	15390801	4
Caelo	Base cream DAC	15390901	1
Caelo	Base cream DAC	15391101	1
Caelo	Base cream DAC	15391201	3
Caelo	Base cream DAC	15419901	3
Caelo	Base cream DAC	15420001	5
Caelo	Base cream DAC	15420201	8
Caelo	Base cream DAC	15420101	2
Caelo	Base cream DAC	15420401	8
Euro OTC	Base cream DAC	15502028-01	1
Caelo	Base cream DAC	1587201	1
Fagron	Base cream DAC	1586	1
Fagron	Base cream DAC	15B19-T13-019450	1
Bombastus	Base cream DAC	15C-11T05-020388	1
Fagron	Base cream DAC	15C11-T07-020396	1
Fagron	Base cream DAC	15C11-T04-020384	2
Fagron	Base cream DAC	15C11-T06-020392	1
Fagron	Base cream DAC	15C11-T05-020388	1
Fagron	Base cream DAC	15C11-T09	1
Fagron	Base cream DAC	15C11-T09-020405	1
Fagron	Base cream DAC	15C11T13020416	1
Fagron	Base cream DAC	15C11-T14-020420	2
Fagron	Base cream DAC	15C11-To4-020384	1
Fagron	Base cream DAC	15H04-T05-024975	4
Caelo	Base cream DAC	15F30-T14-034792	1
Fagron	Base cream DAC	15H04-T06-024978	2
Fagron	Base cream DAC	15C11-T11-020411	1
Fagron	Base cream DAC	15h04-t06-024978	2
Fagron	Base cream DAC	15E27-T02-022881	1
Fagron	Base cream DAC	15H04-T08-024987	2
Fagron	Base cream DAC	15H04-T11-024997	2
Fagron	Base cream DAC	15H04-T10-024994	1
Caelo	Base cream DAC	15J13-T03-026895	1
Fagron	Base cream DAC	15J13-T03-026895	3

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Supplier	Substance	Batch	Spectra
Fagron	Base cream DAC	15H04-T14-025007	1
Fagron	Base cream DAC	15L17-T05-028785	2
Caelo	Base cream DAC	16/078/B	1
Fagron	Base cream DAC	15L17-T06-028791	1
Bombastus	Base cream DAC	16005201	1
Caelo	Base cream DAC	16005101	1
Caelo	Base cream DAC	16005201	2
Euro OTC	Base cream DAC	1601055-01	2
Caelo	Base cream DAC	16005301	3
Caelo	Base cream DAC	160102801	1
Caelo	Base cream DAC	1601023-01	1
Caelo	Base cream DAC	1601027-01	1
Caesar&Loretz	Base cream DAC	16005201	1
Euro OTC	Base cream DAC	1603015-01	1
EuRho/Noweda	Base cream DAC	1603015-01	1
Euro OTC	Base cream DAC	1603016-01	4
Euro OTC	Base cream DAC	1603028-01	9
Euro OTC	Base cream DAC	160301601	1
Euro OTC	Base cream DAC	1603029-01	3
Caelo	Base cream DAC	1603037-01	1
Caelo	Base cream DAC	16041001	1
Euro OTC	Base cream DAC	1603038-01	1
Caelo	Base cream DAC	16055501	1
Phoenix	Base cream DAC	16041301	1
Euro OTC	Base cream DAC	1604042-01	2
Sanacorp 16.07.2016	Base cream DAC	1604023-01	1
Caelo	Base cream DAC	16055701	7
Caelo	Base cream DAC	16055601	3
Noweda	Base cream DAC	16058801	1
Caelo	Base cream DAC	16055801	1
Caelo	Base cream DAC	16055801	1
Caelo	Base cream DAC	16058801	7
Caelo	Base cream DAC	16055901	2
Phytocomm	Base cream DAC	16058801	1
Caelo	Base cream DAC	16061402	1
Caelo	Base cream DAC	16059101	2
Phoenix	Base cream DAC	16059101	1
Caelo	Base cream DAC	16091901	1
Caelo	Base cream DAC	16097601	3
Caelo	Base cream DAC	16101201	5
Caelo	Base cream DAC	16101301	3
Caelo	Base cream DAC	16101901	5
Caelo	Base cream DAC	16101901	1
Caelo	Base cream DAC	16102101	1
Caelo	Base cream DAC	16102201	2
Caelo	Base cream DAC	16103801	2
Caelo	Base cream DAC	16103701	1
Caelo	Base cream DAC	16103901	5
Caelo	Base cream DAC	16104001	1
Caelo	Base cream DAC	16128901	2
Caelo	Base cream DAC	16131501	3
Caelo	Base cream DAC	16131901	5
Caelo	Base cream DAC	16132001	3
Lamotte	Base cream DAC	16132001	1
Caelo	Base cream DAC	16132101	7
Caelo	Base cream DAC	16132201	1
Caelo	Base cream DAC	16134701	6
Caelo	Base cream DAC	16135001	6
Caelo	Base cream DAC	16135701	2
Caelo	Base cream DAC	16135101	1

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Supplier	Substance	Batch	Spectra
Caelo	Base cream DAC	16135801	1
Caelo	Base cream DAC	16136001	3
Caelo	Base cream DAC	16145601	5
Caelo	Base cream DAC	16136301	4
Caelo	Base cream DAC	16145701	7
Caelo	Base cream DAC	16145801	4
Caelo	Base cream DAC	16146001	7
Caelo	Base cream DAC	16145901	1
Caelo	Base cream DAC	16149901	2
Caelo	Base cream DAC	16150301	1
Caelo	Base cream DAC	16152101	1
Caeolo/Noweda	Base cream DAC	16152101	1
Caelo	Base cream DAC	16152401	3
Caelo	Base cream DAC	16155801	1
Caelo	Base cream DAC	16203301	2
Caelo	Base cream DAC	16205501	1
Gehe	Base cream DAC	16205501	1
Phoenix	Base cream DAC	16205601	1
Caelo	Base cream DAC	16206801	3
Caelo	Base cream DAC	16214801	3
Caelo	Base cream DAC	1620901	1
Caelo	Base cream DAC	16219401	1
Caesar&Loretz	Base cream DAC	16219401	1
Caelo	Base cream DAC	16220301	6
Caelo	Base cream DAC	16220201	1
Caelo	Base cream DAC	16220401	7
Gehe	Base cream DAC	16232201	1
Caelo	Base cream DAC	16227101	1
Caelo	Base cream DAC	16231901	1
Caelo	Base cream DAC	16232102	1
Caelo	Base cream DAC	16232001	2
Bombastus	Base cream DAC	16232201	1
Caelo	Base cream DAC	16232301	4
Caelo	Base cream DAC	16232401	3
Caelo	Base cream DAC	16232601	3
Caelo	Base cream DAC	16237901	1
Caelo	Base cream DAC	1623801	1
Caelo	Base cream DAC	16238301	3
Caelo	Base cream DAC	16260701	1
Caelo	Base cream DAC	16241001	3
Caelo	Base cream DAC	16240301	1
PHÖNIX	Base cream DAC	16261002	1
Caelo	Base cream DAC	16260901	1
Caelo	Base cream DAC	16261002	1
Caelo	Base cream DAC	16253101	1
Caelo	Base cream DAC	16240601	1
Caelo	Base cream DAC	16241601	1
Caelo	Base cream DAC	16261101	3
Caelo	Base cream DAC	16262101	1
Caelo	Base cream DAC	16349502	1
Caelo	Base cream DAC	16350301	1
Caelo	Base cream DAC	16352701	2
Caelo	Base cream DAC	16326101	2
Caelo	Base cream DAC	16326001	1
Fagron	Base cream DAC	16815-T04-030282	1
Fagron	Base cream DAC	16A25-T02-029645	1
Caelo	Base cream DAC	1650201	1
Fagron	Base cream DAC	16B15-T01-030274	1
Caelo	Base cream DAC	16B15-T02-030277	2
Caelo	Base cream DAC	16B15-T04-030281	4

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Supplier	Substance	Batch	Spectra
Fagron	Base cream DAC	16B15-T02-030277	1
Fagron	Base cream DAC	16B15-T04-030281	2
Fagron	Base cream DAC	16C24-T05031490	1
Caelo	Base cream DAC	16F30-T13-034789	1
Fagron	Base cream DAC	16C24-T06-031494	1
Fagron	Base cream DAC	16B15-T04-030282	1
Fagron	Base cream DAC	16D06-T09-031941	1
Caelo	Base cream DAC	16F30-T14-034792	1
Fagron	Base cream DAC	16G20-T04-035305	2
Caelo	Base cream DAC	19081503	1
Caelo	Base cream DAC	17006501	1
Caelo	Base cream DAC	17003401	1
Caelo	Base cream DAC	21081407	1
Caelo	Base cream DAC	170216Vi4	1
Caelo	Base cream DAC	20021503	1
Caelo	Base cream DAC	180615010	1
Noweda/Ensbona	Base cream DAC	222512	1
Ensbona/Sanacorp	Base cream DAC	22251214	2
Caelo	Base cream DAC	23041403	1
Eimermacher	Base cream DAC	23090414	1
Caelo	Base cream DAC	23061506	1
Bombastus	Base cream DAC		4
Noweda/Ensbona	Base cream DAC	24180414	4
Caelo	Base cream DAC	2514U1309	1
Bombastus	Base cream DAC	260416v3	1
Bombastus	Base cream DAC	278398	5
Bombastus	Base cream DAC	280078	2
Caelo	Base cream DAC	26091405	1
Bombastus	Base cream DAC	281243	2
Bombastus	Base cream DAC	279962	1
Caelo	Base cream DAC	26011602	1
Bombastus	Base cream DAC	282773	1
Bombastus	Base cream DAC	283918	1
gehe	Base cream DAC	283915	1
Euro OTC	Base cream DAC	281486	1
Bombastus	Base cream DAC	283972	2
Bombastus	Base cream DAC	283973	1
Bombastus	Base cream DAC	283976	1
Bombastus	Base cream DAC	283975	1
Bombastus	Base cream DAC	283974	2
Bombastus	Base cream DAC	285228	4
Bombastus	Base cream DAC	285227	1
Bombastus	Base cream DAC	286087	4
Bombastus	Base cream DAC	286088	3
Bombastus	Base cream DAC	286089	1
Bombastus	Base cream DAC	286094	3
Bombastus	Base cream DAC	286093	2
Bombastus	Base cream DAC	286090	2
Bombastus	Base cream DAC	286155	2
Bombastus	Base cream DAC	286158	3
Fagron	Base cream DAC	286157	1
Bombastus	Base cream DAC	286159	1
Bombastus	Base cream DAC	286160	2
Bombastus	Base cream DAC	286162	1
Bombastus	Base cream DAC	287110	1
Bombastus	Base cream DAC	287112	1
Bombastus	Base cream DAC	287114	1
Bombastus	Base cream DAC	287115	2
Bombastus	Base cream DAC	287116	2
Bombastus	Base cream DAC	287117	1

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Supplier	Substance	Batch	Spectra
Bombastus	Base cream DAC	287197	5
Bombastus	Base cream DAC	287248	2
Fagron	Base cream DAC	287197	1
Bombastus	Base cream DAC	287196	1
Gehe	Base cream DAC	287249	1
Bombastus	Base cream DAC	287876	1
Bombastus	Base cream DAC	287875	2
Bombastus	Base cream DAC	287251	2
Caelo	Base cream DAC	287876	1
Gehe	Base cream DAC	287868	1
Bombastus	Base cream DAC	287944	1
Bombastus	Base cream DAC	287941	1
Bombastus	Base cream DAC	287946	2
Bombastus	Base cream DAC	288054	1
Bombastus	Base cream DAC	288055	3
Gehe	Base cream DAC	287947	1
Bombastus	Base cream DAC	289530	1
Bombastus	Base cream DAC	289526	2
Bombastus	Base cream DAC	289531	1
Bombastus	Base cream DAC	289589	1
Bombastus	Base cream DAC	289590	1
Bombastus	Base cream DAC	289663	2
Sonnenberg-Apotheke	Base cream DAC	289663	1
Bombastus	Base cream DAC	289665	1
Bombastus	Base cream DAC	289667	2
Bombastus	Base cream DAC	289669	1
Bombastus	Base cream DAC	289803	1
Bombastus	Base cream DAC	289804	1
Bombastus	Base cream DAC	289805	1
Bombastus	Base cream DAC	291024	1
Gehe	Base cream DAC	291025	1
Bombastus	Base cream DAC	291025	2
Bombastus	Base cream DAC	291029	1
Bombastus	Base cream DAC	291026	3
Bombastus	Base cream DAC	291028	1
Bombastus	Base cream DAC	292125	4
Bombastus	Base cream DAC	291069	1
Bombastus	Base cream DAC	292127	1
Bombastus	Base cream DAC	292123	1
Bombastus	Base cream DAC	292122	1
Ensbona/Sanacorp	Base cream DAC	29220416	1
Bombastus	Base cream DAC	292260	2
Bombastus	Base cream DAC	292259	1
Bombastus	Base cream DAC	292267	2
Bombastus	Base cream DAC	292263	1
Ensbona/Eimermacher	Base cream DAC	29230416	1
Bombastus	Base cream DAC	293196	1
Bombastus	Base cream DAC	293197	1
Bombastus	Base cream DAC	293201	1
Bombastus	Base cream DAC	293795	3
Bombastus	Base cream DAC	293200	1
Bombastus	Base cream DAC	293939	3
Bombastus	Base cream DAC	293796	1
Bombastus	Base cream DAC	293940	1
Bombastus	Base cream DAC	293973	1
Bombastus	Base cream DAC	294839	1
Bombastus	Base cream DAC	294836	1
Bombastus	Base cream DAC	295899	1
Bombastus	Base cream DAC	294842	2
Bombastus	Base cream DAC	294843	2

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Supplier	Substance	Batch	Spectra
Bombastus	Base cream DAC	295897	3
Bombastus	Base cream DAC	295900	1
Bombastus	Base cream DAC	295901	1
Bombastus	Base cream DAC	296155	1
Bombastus	Base cream DAC	296226	2
Bombastus	Base cream DAC	296224	1
Bombastus	Base cream DAC	296227	1
Bombastus	Base cream DAC	296229	3
Bombastus	Base cream DAC	296228	1
Bombastus	Base cream DAC	297484	1
Bombastus	Base cream DAC	297480	1
Bombastus	Base cream DAC	297494	4
Bombastus	Base cream DAC	297500	1
Bombastus	Base cream DAC	298171	1
Bombastus	Base cream DAC	298170	1
Bombastus	Base cream DAC	298173	2
Bombastus	Base cream DAC	298256	1
Bombastus	Base cream DAC	298257	1
Caelo	Base cream DAC	298259	2
Bombastus	Base cream DAC	298259	3
Bombastus	Base cream DAC	298260	1
Bombastus	Base cream DAC	298262	2
Bombastus	Base cream DAC	299322	2
Caelo	Base cream DAC	298260	1
Bombastus	Base cream DAC	299320	2
Bombastus	Base cream DAC	298265	1
Bombastus	Base cream DAC	299323	3
Bombastus	Base cream DAC	299947	1
Bombastus	Base cream DAC	300014	3
Caelo	Base cream DAC	299323	1
Bombastus	Base cream DAC	301148	1
Bombastus	Base cream DAC	301155	2
Bombastus	Base cream DAC	301159	3
Caelo	Base cream DAC	301157	1
Bombastus	Base cream DAC	301160	1
Caelo	Base cream DAC	301743	2
Bombastus	Base cream DAC	301741	1
Bombastus	Base cream DAC	301758	2
Bombastus	Base cream DAC	301759	2
Bombastus	Base cream DAC	303061	2
Bombastus	Base cream DAC	303062	1
Caelo	Base cream DAC	303061	1
Alliance Healthcare	Base cream DAC	303417	1
Caelo	Base cream DAC	303058	1
Bomastus/Phönix	Base cream DAC	303423	4
Caelo	Base cream DAC	303419	1
Bombastus	Base cream DAC	303425	1
Bombastus	Base cream DAC	304351	1
Bombastus	Base cream DAC	304342	1
Bombastus	Base cream DAC	304352	1
Bombastus	Base cream DAC	304353	1
Caelo	Base cream DAC	304352	1
Bombastus	Base cream DAC	304359	1
Bombastus	Base cream DAC	304360	1
Caelo	Base cream DAC	31031405	1
Caelo	Base cream DAC	31031506	1
Euro OTC	Base cream DAC	38540516	3
PKH GmbH	Base cream DAC	34567890	1
Caesar & Loretz/AHC	Base cream DAC	38540516	3
Euro OTC	Base cream DAC	3854056	1

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Supplier	Substance	Batch	Spectra
Caelo	Base cream DAC	39210516	1
P.W.Beyvers	Base cream DAC	412/1	2
Gehe am 08.04.2014	Base cream DAC	412/1	2
P.W.Beyvers GmbH/Anzag	Base cream DAC	412/2	1
Noweda / Beyvers	Base cream DAC	412/2	1
P.W.Beyvers	Base cream DAC	440/1	1
Fagron	Base cream DAC	412/2	2
Caelo	Base cream DAC	412/2	1
Caelo	Base cream DAC	412/3	1
P.W.Beyvers	Base cream DAC	412/3	1
Stumpf/Beyvers	Base cream DAC	412/2	1
Beyvers	Base cream DAC	440/1	1
Noweda/Beyvers	Base cream DAC	412/3	2
Beyvers	Base cream DAC	440/2	1
P.W.Beyvers	Base cream DAC	440/2	1
Euro OTC	Base cream DAC	44950616	12
Gehe/Beyvers	Base cream DAC	440/2	1
Euro OTC	Base cream DAC	44960616	2
Euro OTC	Base cream DAC	45330616	10
Ensbona/Eimermacher	Base cream DAC	45150616	1
Euro OTC	Base cream DAC	45340616	4
Caelo	Base cream DAC	45348616	1
Caelo	Base cream DAC	45380616	2
Eurho/Noweda	Base cream DAC	45380616	1
Euro OTC	Base cream DAC	45380616	3
Ensbona/Anzag	Base cream DAC	50211015	4
Euro OTC	Base cream DAC	49650616	1
Eimermacher	Base cream DAC	50221015	1
Ensbona/ Sanacorp	Base cream DAC	50211015	1
Phönix Gotha	Base cream DAC	515/1	1
Caelo	Base cream DAC	50205/1Gra	1
P.W.Beyvers GmbH / Noweda	Base cream DAC	515/3	1
P.W. Beyvers GmbH/Phönix	Base cream DAC	515/2	2
P.W.Beyvers GmbH/ Sanac...	Base cream DAC	515/2	1
Beyvers	Base cream DAC	5153	1
Phönix Gotha	Base cream DAC	515/3	1
Phönix Gotha	Base cream DAC	538/1	1
P.W. Beyvers GmbH / Phö...	Base cream DAC	538/1	2
Beyvers	Base cream DAC	538/1	2
Beyvers	Base cream DAC	538-1	1
Beyvers/ Phönix	Base cream DAC	538/2	1
Lamotte/ AHDE	Base cream DAC	5407700	1
Beyvers	Base cream DAC	538/2	1
Henry Lamotte	Base cream DAC	5489900	2
Lamotte/AHD	Base cream DAC	5490000	2
Euro OTC	Base cream DAC	55360616	2
Sanacorp	Base cream DAC	5537000	2
Lamotte/Noweda	Base cream DAC	553700	1
Henry Lamotte Oils GmbH	Base cream DAC	5537000	12
Caelo	Base cream DAC	5537000	8
Fagron	Base cream DAC	5537000	1
Lamotte	Base cream DAC	5537300	3
Phönix Gotha	Base cream DAC	5537100	1
Phoenix 24.03.2014	Base cream DAC	5537200	2
Phönix Gotha	Base cream DAC	5537300	1
Lamotte/Alliance	Base cream DAC	5537500	2
Lamotte/Alliance	Base cream DAC	5537600	1
Henry Lamotte/Anzag	Base cream DAC	5537600	2
Henry Lamotte Oils/Sana...	Base cream DAC	5650600	1
AHD	Base cream DAC	5650700	5

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Supplier	Substance	Batch	Spectra
HenryLamotteGmbH/Noweda	Base cream DAC	5650800	1
Phönix Gotha	Base cream DAC	5650900	1
Phönix Gotha	Base cream DAC	5650600	1
lamotte/sanacorb	Base cream DAC	5651000	2
Henry Lamotte Olis GmbH	Base cream DAC	5651100	1
Phoenix	Base cream DAC	5651300	2
Lamotte/Anzag	Base cream DAC	5651100	1
henry lamotte oils gmbh	Base cream DAC	5650900	1
Henry Lamotte/Anzag	Base cream DAC	5651200	1
Lamotte/Alliance	Base cream DAC	5651300	1
Noweda/Ensbona	Base cream DAC	56590714	5
Eimermacher	Base cream DAC	57080315	1
Ensbona/Sanacorp	Base cream DAC	57090315	3
Noweda/Ensbona	Base cream DAC	57090315	1
lamotte/sanacorb	Base cream DAC	5787800	1
Phönix Gotha	Base cream DAC	5787900	1
Henry Lamotte/Anzag	Base cream DAC	5788600	1
Lamotte//AHD	Base cream DAC	5787900	1
Caelo	Base cream DAC	5788000	1
Phönix Gotha	Base cream DAC	5788000	1
Henry Lamotte Oils / No...	Base cream DAC	5788200	1
Henry Lamotte Oils/Phönix	Base cream DAC	5788700	2
Caelo	Base cream DAC	5788100	1
Henry Lamotte/Anzag	Base cream DAC	5788700	3
Caelo	Base cream DAC	5909200	1
Henry Lamotte Oils GmbH	Base cream DAC	5909400	1
Sanacorp/Henry Lamotte	Base cream DAC	5909300	1
Caelo	Base cream DAC	5909300	1
Caelo	Base cream DAC	5909500	1
Henry Lamotte /Noveda	Base cream DAC	5909600	1
Henry Lamotte/Anzag	Base cream DAC	5909500	1
Henry Lamotte Oils GmbH	Base cream DAC	5909600	1
Henry Lamotte Oils / No...	Base cream DAC	5909500	1
Lamotte/Phönix	Base cream DAC	5909600	1
Lamotte	Base cream DAC	590990	1
Lamotte/AHD	Base cream DAC	5909600	1
Anzag/Lamotte	Base cream DAC	591000	1
Caelo	Base cream DAC	6002237002	1
Lamotte/Gehe	Base cream DAC	6002237002	1
Henry Lamotte/Anzag	Base cream DAC	5909800	1
Sana/Henry Lamotte	Base cream DAC	6002237003	1
Lamotte//AHD	Base cream DAC	6002237004	1
Lamotte/ANZAG	Base cream DAC	6002237008	1
Henry Lamotte/Anzag	Base cream DAC	6002237009	2
Henry Lamotte Oils GmbH	Base cream DAC	6002237002	1
Lamotte/AHD	Base cream DAC	600237004	1
Henry Lamotte/AHD	Base cream DAC	6002237005	2
Lamotte/AHD	Base cream DAC	6002237006	1
Henry Lamotte Oils / No...	Base cream DAC	6002237005	1
Caelo	Base cream DAC	6003682004	1
Lamotte/ Anzag	Base cream DAC	6003682005	1
mephano	Base cream DAC	6500115	2
Beyvers	Base cream DAC	640/2	1
Sanacorp	Base cream DAC	75/AKD4	1
Caelo	Base cream DAC	74/AKD2	1
Euro OTC	Base cream DAC	91310916	1
Sanacorp	Base cream DAC	72/AKD2	1
Lamotte/AHD	Base cream DAC	6003682013	1
Sanacorp	Base cream DAC	75/AKD6	1
Euro OTC	Base cream DAC	701228	1

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Supplier	Substance	Batch	Spectra
Gehe	Base cream DAC	cdbgsdgb	1
Caelo	Base cream DAC		14
Bombastus	Base cream DAC	CHB289803	1
/ Anzag	Base cream DAC		1
Ensbona/ Sanacorp	Base cream DAC		2
Bombastus	Base cream DAC	265036	2
Bombastus	Base cream DAC	263291	1
Bombastus	Base cream DAC	263423	1
Bombastus	Base cream DAC	265029	1
Bombastus	Base cream DAC	263429	1
Bombastus	Base cream DAC	266637	3
Gehe	Base cream DAC	266525	1
Gehe	Base cream DAC	266663	1
Bombastus	Base cream DAC	266749	1
Bombastus	Base cream DAC	266752	1
Bombastus	Base cream DAC	268815	2
Bombastus	Base cream DAC	268925	6
Caelo	Base cream DAC	268820	2
Anzag 27.08.2012	Base cream DAC	268819	1
Bombastus	Base cream DAC	266799	1
Bombastus	Base cream DAC	268821	1
Bombastus	Base cream DAC	269996	1
PHOENIX am 08.06.2012	Base cream DAC	269997	1
Bombastus	Base cream DAC	270000	3
Bombastus	Base cream DAC	270157	1
Bombastus	Base cream DAC	272001	1
Bombastus	Base cream DAC	271999	1
Caelo	Base cream DAC	272084	2
Bombastus	Base cream DAC	272084	4
Gehe	Base cream DAC	272000	1
Bombastus	Base cream DAC	272086	2
Phoenix	Base cream DAC	272091	1
Bombastus	Base cream DAC	272091	1
Bombastus	Base cream DAC	272093	1
Bombastus	Base cream DAC	272215	4
Bombastus	Base cream DAC	272216	1
Anzag 09.11.12	Base cream DAC	272216	1
Phönix 22.11.12	Base cream DAC	272218	1
Phoenix	Base cream DAC	272219	2
Bombastus	Base cream DAC	272219	1
Bombastus	Base cream DAC	272221	1
Bombastus	Base cream DAC	272464	3
Eimermacher	Base cream DAC	2770713	1
Caelo	Base cream DAC	1061303	1
Caelo	Base cream DAC	3121302	1
Caelo	Base cream DAC	1081302	1
Gehe	Base cream DAC	4A131113	1
Caelo	Base cream DAC	213M-01309	1
Caelo	Base cream DAC	5091308	1
KEHR / Beyvers GmbH	Base cream DAC	71112PML01	1
Caelo	Base cream DAC	513Q-01309	1
Caelo	Base cream DAC	713I-01309	1
Caelo	Base cream DAC	8111302	1
Euro OTC	Base cream DAC	80616-8	1
Caelo	Base cream DAC	8011302	1
Caelo	Base cream DAC	913I-01309	1
Caelo	Base cream DAC	1013Q-01309	3
Noweda	Base cream DAC	11/30-T01	5
Caelo	Base cream DAC	1004211309	1
Caelo	Base cream DAC	11011405	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Base cream DAC	1107040-01	1
Caelo	Base cream DAC	11087101	1
EuRho	Base cream DAC	1108002-01	1
Euro OTC	Base cream DAC	11033-01	1
Caelo	Base cream DAC	1109211309	1
Caelo	Base cream DAC	11101302	1
Euro OTC	Base cream DAC	1110037-01	2
Euro OTC	Base cream DAC	11110023-01	1
Euro OTC	Base cream DAC	1111009-01	1
EuRho Anzag ek:33,16 03. ...	Base cream DAC	1111027-01	1
Euro OTC	Base cream DAC	1111028-01	1
Europharm/Otto	Base cream DAC	1111028-01	2
Phönix	Base cream DAC	1111029-01	1
Euro OTC	Base cream DAC	1111041-01	1
Caelo	Base cream DAC	11206201	3
Euro OTC	Base cream DAC	1111051-01	2
EuRho	Base cream DAC	1111050-01	1
EuRho	Base cream DAC	1111048-01	1
Caelo	Base cream DAC	11279001	2
Caelo	Base cream DAC	11278701	1
Noweda	Base cream DAC	11229001	1
Gehe	Base cream DAC	111105101	1
Caesar & Loretz GmbH, 4. ...	Base cream DAC	11278901	1
Caelo	Base cream DAC	11279401	1
Caelo	Base cream DAC	11295801	2
Caesar & Loretz	Base cream DAC	11296701	1
Caelo	Base cream DAC	11296301	1
Caelo	Base cream DAC	11296501	1
Caelo	Base cream DAC	11295701	1
Caelo	Base cream DAC	11296601	1
Caelo	Base cream DAC	11297201	9
Caelo	Base cream DAC	11296901	1
Caelo	Base cream DAC	11296701	1
Caelo	Base cream DAC	11297001	1
Caelo	Base cream DAC	11297301	1
Fagron	Base cream DAC	11297301	1
Kehr	Base cream DAC	1130501	1
Caelo	Base cream DAC	11330101	2
Caelo	Base cream DAC	11330201	1
Fagron	Base cream DAC	1130-T01	1
Noweda	Base cream DAC	11K06-T01	5
Fagron	Base cream DAC	11B11-T05	4
Caelo	Base cream DAC	11330401	1
Caelo	Base cream DAC	11330301	1
Caelo	Base cream DAC	11330601	1
Fagron	Base cream DAC	11K06-T01	1
Noweda	Base cream DAC	11130-t01	1
Noweda	Base cream DAC	11130-T01	1
Caelo	Base cream DAC	12000501	3
Caelo	Base cream DAC	12000401	2
Caelo	Base cream DAC	12000101	1
Caelo	Base cream DAC	12000601	1
Caelo	Base cream DAC	12005101	3
Caelo	Base cream DAC	12004901	2
Caelo	Base cream DAC	12005201	2
Caelo	Base cream DAC	12005501	5
Caelo	Base cream DAC	12005401	1
Noweda	Base cream DAC	12005601	1
Caelo	Base cream DAC	12005701	6
Kehr	Base cream DAC	12005601	1

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Supplier	Substance	Batch	Spectra
Doroderm GmbH/ Noweda	Base cream DAC	1202001	4
doroderm GmbH	Base cream DAC	1202001	2
Sanacorp	Base cream DAC	1202001	3
Caelo	Base cream DAC	1202001	2
Euro OTC	Base cream DAC	1204004-01	3
Euro OTC	Base cream DAC	1204024-01	1
Euro OTC	Base cream DAC	1204025-01	2
Anzag 25.10.12 ek:33,15EUR	Base cream DAC	1205005-01	1
Euro OTC	Base cream DAC	1204023-01	1
Euro OTC	Base cream DAC	1205007-01	2
Klenk	Base cream DAC	1205004-01	1
Euro OTC	Base cream DAC	1205018-01	3
Euro OTC	Base cream DAC	1205040-01	1
Euro OTC	Base cream DAC	1205019-01	1
Euro OTC	Base cream DAC	1205044-01	2
Euro OTC	Base cream DAC	1205041-01	1
DAC 2011	Base cream DAC	12061901	1
Caelo	Base cream DAC	12062001	2
Caesar & Loretz GmbH, 4...	Base cream DAC	12062601	1
Caelo	Base cream DAC	12061601	1
Caelo	Base cream DAC	12061701	1
Euro OTC	Base cream DAC	1205043-01	1
Caelo	Base cream DAC	12062601	2
Caelo	Base cream DAC	12062701	2
Caelo	Base cream DAC	12062801	2
Caelo	Base cream DAC	12063001	3
Caelo	Base cream DAC	12063101	1
Caelo	Base cream DAC	12062901	1
Euro OTC	Base cream DAC	1209037-01	2
Caelo	Base cream DAC	12071202	1
EuRho	Base cream DAC	1209037-01	1
Euro OTC	Base cream DAC	1209038-01	2
Euro OTC	Base cream DAC	120903701	1
Anzag 14.01.2013	Base cream DAC	1210011-01	1
Euro OTC	Base cream DAC	1210011-01	3
Euro OTC	Base cream DAC	1210044-01	4
Euro OTC	Base cream DAC	1210055-01	3
Euro OTC	Base cream DAC	1210054-01	1
Euro OTC	Base cream DAC	121005401	1
Euro OTC	Base cream DAC	1210053-01	1
Hirsch	Base cream DAC	1210054-01	1
Caelo	Base cream DAC	12116001	1
Caelo	Base cream DAC	12101203	1
Caelo	Base cream DAC	12111202	1
AHC 27.06.13 EK 32,95	Base cream DAC	1212025-01	1
Euro OTC	Base cream DAC	1212025-01	1
anzag 29.01.13 ek: 33,15EUR	Base cream DAC	1212027-01	1
Euro OTC	Base cream DAC	1212028-01	2
Euro OTC	Base cream DAC	121202801	1
Bombastus	Base cream DAC	1212029-01	3
Euro OTC	Base cream DAC	121209-01	1
Caelo	Base cream DAC	12159301	2
Caelo	Base cream DAC	1213M-01309	1
Caelo	Base cream DAC	12159401	2
Caelo	Base cream DAC	12159201	1
Caelo	Base cream DAC	12159601	5
Caelo	Base cream DAC	12167901	12
Caelo	Base cream DAC	12168001	2
Caelo	Base cream DAC	12168101	2
Caelo	Base cream DAC	12168201	1

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Supplier	Substance	Batch	Spectra
Caelo	Base cream DAC	12168301	1
Kehr	Base cream DAC	12168301	1
Caelo	Base cream DAC	12174801	3
Caelo	Base cream DAC	12174901	3
Finze	Base cream DAC	12174901	1
Caelo	Base cream DAC	12175001	5
Caelo	Base cream DAC	12175101	1
Caelo	Base cream DAC	12175201	2
Caelo	Base cream DAC	12178301	4
Cealo/Gehe	Base cream DAC	12175101	1
Caelo	Base cream DAC	12178401	3
Caelo	Base cream DAC	12191701	3
Caelo	Base cream DAC	12191801	5
Infecto/Phönix	Base cream DAC	12191901	1
Caelo	Base cream DAC	12191902	1
Caelo	Base cream DAC	12192001	2
Caelo	Base cream DAC	12192201	2
Hersteller: Beyvers	Base cream DAC	122/1	1
Caelo	Base cream DAC	12192101	1
Caelo	Base cream DAC	12240801	2
Caelo	Base cream DAC	12240901	5
Noweda	Base cream DAC	12240801	1
Caelo	Base cream DAC	12241001	5
Caelo	Base cream DAC	12241201	1
phönix, 13.11.2012	Base cream DAC	12241201	1
Caelo	Base cream DAC	12241101	1
Caelo	Base cream DAC	12245001	2
Erika apotheke	Base cream DAC	1224501	1
anzag, 20.11.2012	Base cream DAC	12245001	1
Caelo	Base cream DAC	12245201	1
Cealo	Base cream DAC	12249401	1
Caelo	Base cream DAC	12249401	3
Caelo	Base cream DAC	12245101	2
Caelo	Base cream DAC	12249701	2
Caelo	Base cream DAC	12262501	5
Caelo	Base cream DAC	12262402	3
Caelo	Base cream DAC	12262601	3
Caelo	Base cream DAC	12262801	6
Caelo	Base cream DAC	12262901	3
Caelo	Base cream DAC	1226290	1
Sanacorp	Base cream DAC	12262801	1
Gehe	Base cream DAC	12262901	1
Phönix	Base cream DAC	12262901	1
Sanacorp	Base cream DAC	12263001	1
Caelo	Base cream DAC	12263001	1
Kehr	Base cream DAC	12263101	1
Caelo	Base cream DAC	12263101	4
Caelo	Base cream DAC	12263201	6
Caelo	Base cream DAC	12263301	2
Caelo	Base cream DAC	12263401	5
Caelo	Base cream DAC	12289701	4
Phönix 01.02.13	Base cream DAC	12263201	1
Sanacorp	Base cream DAC	12289701	1
Noweda	Base cream DAC	12263501	1
Sanacorp	Base cream DAC	12304701	1
Caelo	Base cream DAC	12303901	3
Caelo	Base cream DAC	12304701	10
Caelo	Base cream DAC	12304801	9
Kehr	Base cream DAC	12304801	1
Phönix	Base cream DAC	12304801	3

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Supplier	Substance	Batch	Spectra
Sanacorp	Base cream DAC	12304901	2
Caelo	Base cream DAC	12305001	5
Caelo	Base cream DAC	12304901	3
Caelo	Base cream DAC	12305101	1
Caelo	Base cream DAC	12305301	4
Alliance Healthcare	Base cream DAC	12305301	1
Caelo	Base cream DAC	12339101	2
Caelo	Base cream DAC	12339001	2
Caesar & Loretz GmbH, 4...	Base cream DAC	12339101	1
Caelo	Base cream DAC	12339201	8
Sanacorp	Base cream DAC	12339001	1
Noweda	Base cream DAC	12339201	1
Krieger	Base cream DAC	12339301	1
Caelo	Base cream DAC	12339301	4
Euro OTC	Base cream DAC	12339301	1
Caelo	Base cream DAC	12339401	6
Caelo	Base cream DAC	12343801	5
Caelo	Base cream DAC	12347101	2
Caelo	Base cream DAC	12347301	5
Caelo	Base cream DAC	12347401	5
Gehe	Base cream DAC	12347301	1
Euro OTC	Base cream DAC	129037-01	1
Caelo	Base cream DAC	12384002	2
Caelo	Base cream DAC	1239201	1
Caelo	Base cream DAC	125044-1	1
Fagron	Base cream DAC	12C02-T08	5
Großhandel	Base cream DAC	12C26-T08	1
Fagron	Base cream DAC	12C26-T04	1
Fagron	Base cream DAC	12C02-T08	1
Fagron	Base cream DAC	12G25T03	1
Fagron	Base cream DAC	12C26-T14	1
Fagron	Base cream DAC	12C26-T08	2
Fagron	Base cream DAC	12G25-T03	3
Fagron	Base cream DAC	12G25-T04	3
Fagron	Base cream DAC	12G25-T06	2
Noweda	Base cream DAC	12G25-T04	1
Fagron	Base cream DAC	12G25-T12	2
Fagron	Base cream DAC	12G25-T10	1
Caelo	Base cream DAC	13000701	2
Caelo	Base cream DAC	13000601	1
Caelo	Base cream DAC	130000601	1
Phönix	Base cream DAC	13000601	1
Phönix	Base cream DAC	13000701	1
Caelo	Base cream DAC	13000501	1
Caelo	Base cream DAC	13000801	2
Caelo	Base cream DAC	13000901	1
Caelo	Base cream DAC	13007001	4
Caelo	Base cream DAC	13007101	6
Phönix	Base cream DAC	13007101	1
phönix	Base cream DAC	13007101	1
Caelo	Base cream DAC	13007201	3
Caelo	Base cream DAC	13007301	2
EuRho	Base cream DAC	1301022-01	2
Euro OTC	Base cream DAC	130102301	1
EuRho	Base cream DAC	1301023-01	1
Euro OTC	Base cream DAC	1301040-01	1
Euro OTC	Base cream DAC	1301042-01	1
Euro OTC	Base cream DAC	1301043-01	1
Euro OTC	Base cream DAC	1301044-01	1
Caelo	Base cream DAC	13012401	10

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Supplier	Substance	Batch	Spectra
calo	Base cream DAC	13012401	1
Caelo	Base cream DAC	13012601	2
Caelo	Base cream DAC	13012501	3
Caelo	Base cream DAC	13016901	3
Caelo	Base cream DAC	13016801	1
Caelo	Base cream DAC	13017001	3
Caelo	Base cream DAC	13017101	1
Caelo	Base cream DAC	1301681	1
Caelo	Base cream DAC	13017201	3
Euro OTC	Base cream DAC	1302037-01	2
EuRho	Base cream DAC	1302036-01	1
Euro OTC	Base cream DAC	1304004-01	2
EuRho	Base cream DAC	1302009-01	1
Caelo	Base cream DAC	13022401	1
Euro OTC	Base cream DAC	130201001	2
Euro OTC	Base cream DAC	1304005-01	2
EuRho	Base cream DAC	130400501	1
Euro OTC	Base cream DAC	1305012-01	2
Euro OTC	Base cream DAC	1304006-01	2
Euro OTC	Base cream DAC	1306001-01	6
Euro OTC	Base cream DAC	1306002-01	1
Euro OTC	Base cream DAC	1306007-01	1
Euro OTC	Base cream DAC	1306008-01	3
Euro OTC	Base cream DAC	1306009-01	2
Euro OTC	Base cream DAC	1306019-01	2
Euro OTC	Base cream DAC	1306020-01	7
Euro OTC	Base cream DAC	130603001	1
Euro OTC	Base cream DAC	1306031-01	1
Caelo	Base cream DAC	1306031-01	1
Euro OTC	Base cream DAC	1306044-01	2
Gehe	Base cream DAC	1306044-01	1
Euro OTC	Base cream DAC	1307031-01	4
Euro OTC	Base cream DAC	130703101	1
Euro OTC	Base cream DAC	130703601	2
Caelo	Base cream DAC	130704501	1
Euro OTC	Base cream DAC	1307035-01	1
Euro OTC	Base cream DAC	1308011-01	1
Euro OTC	Base cream DAC	1307046-01	1
Euro OTC	Base cream DAC	1308021-01	2
Caelo	Base cream DAC	13082101	10
Euro OTC	Base cream DAC	130704801	1
Euro OTC	Base cream DAC	130802-01	1
Caelo	Base cream DAC	13082203	9
Caelo	Base cream DAC	13083101	3
Euro OTC	Base cream DAC	1309005-01	3
Euro OTC	Base cream DAC	1311007-01	2
Euro OTC	Base cream DAC	131100901	1
Euro OTC	Base cream DAC	1311031-01	1
Caelo	Base cream DAC	13111101	3
Caelo	Base cream DAC	13111201	4
Euro OTC	Base cream DAC	1311009-01	1
Caelo	Base cream DAC	13111301	5
Euro OTC	Base cream DAC	13113101	1
Caelo	Base cream DAC	13111401	2
Phönix	Base cream DAC	13111401	2
Caelo	Base cream DAC	13115601	7
Caelo	Base cream DAC	13115701	3
Caelo	Base cream DAC	13115801	4
Caelo	Base cream DAC	13115901	3
Caelo	Base cream DAC	13116001	2

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Supplier	Substance	Batch	Spectra
Caelo	Base cream DAC	13119901	1
Caelo	Base cream DAC	13120001	1
Euro OTC	Base cream DAC	1312001-01	2
Caelo	Base cream DAC	13120101	4
Caelo	Base cream DAC	13120201	3
Caelo	Base cream DAC	13120301	7
Caelo	Base cream DAC	13139702	10
Caelo	Base cream DAC	13125001	4
Caelo	Base cream DAC	13125101	2
Caesar & Loretz GmbH, 4...	Base cream DAC	13139702	1
Noweda	Base cream DAC	13139702	1
Alliance Healthcare	Base cream DAC	13139801	1
Noweda	Base cream DAC	13139901	1
Caesar /phönix	Base cream DAC	13139901	2
Caelo	Base cream DAC	13140001	4
Caelo	Base cream DAC	1315601	1
Caelo	Base cream DAC	13158401	1
Caelo	Base cream DAC	13158440	1
Caelo	Base cream DAC	13158501	9
Caelo	Base cream DAC	13158601	4
Caelo	Base cream DAC	13158801	3
Caelo	Base cream DAC	13173601	14
Caelo	Base cream DAC	13173301	1
Herstellung	Base cream DAC	13173601	1
Sanacorp	Base cream DAC	13173601	1
Sanacorp	Base cream DAC	13173701	1
Caelo	Base cream DAC	13173701	5
Caelo	Base cream DAC	1318701	1
Caelo	Base cream DAC	13187701	2
Caelo	Base cream DAC	13187801	15
Caelo	Base cream DAC	13187901	10
Caelo	Base cream DAC	13188001	6
Caelo	Base cream DAC	13188101	3
Caelo	Base cream DAC	13188401	5
Alliance Healthcare	Base cream DAC	13188101	1
DAC 2011	Base cream DAC	13188401	1
Caelo	Base cream DAC	13188501	9
Caelo	Base cream DAC	13188601	4
Caelo	Base cream DAC	13188701	7
Sanacorp	Base cream DAC	13188801	1
Caelo	Base cream DAC	13188801	2
Caelo	Base cream DAC	1319702	1
Caelo	Base cream DAC	13198501	2
Caelo	Base cream DAC	13198601	8
Noweda	Base cream DAC	13198601	2
Caelo	Base cream DAC	13198801	20
Caelo	Base cream DAC	13198901	8
Caelo	Base cream DAC	13199001	11
Caelo	Base cream DAC	13199101	19
Sanacorp	Base cream DAC	13199101	3
Gehe	Base cream DAC	13199101	1
Euro OTC	Base cream DAC	13201101	1
Caelo	Base cream DAC	132011-01	1
Caelo	Base cream DAC	13249702	3
Caelo	Base cream DAC	13249801	3
Caelo	Base cream DAC	13249901	2
Sanacorp	Base cream DAC	13250001	1
Caelo	Base cream DAC	13250001	8
Fagron	Base cream DAC	13249901	1
Caelo	Base cream DAC	13252101	3

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Supplier	Substance	Batch	Spectra
Caelo	Base cream DAC	13310901	6
Gehe	Base cream DAC	13310901	1
Caelo	Base cream DAC	13311201	9
Caelo	Base cream DAC	13311101	2
Caelo	Base cream DAC	13311301	10
Sanacorp	Base cream DAC	13311301	2
Caelo	Base cream DAC	13311502	1
Caelo	Base cream DAC	13311606	1
Caelo	Base cream DAC	13311601	3
Fagron	Base cream DAC	13311701	1
Phönix	Base cream DAC	13311801	1
Caelo	Base cream DAC	13311701	2
Sanacorp	Base cream DAC	13312001	1
Caelo	Base cream DAC	13312201	3
Caelo	Base cream DAC	1331201	1
Caelo	Base cream DAC	13312101	2
Sanacorp	Base cream DAC	13312301	1
Caelo	Base cream DAC	13312301	4
Caelo	Base cream DAC	13312401	2
Caelo	Base cream DAC	1331801	1
Sanacorp	Base cream DAC	13377201	1
Fagron	Base cream DAC	13378001	2
Caelo	Base cream DAC	13378101	5
Sanacorp	Base cream DAC	13380901	1
Sanacorp	Base cream DAC	13381101	1
Sanacorp	Base cream DAC	13381001	1
D'oroderm	Base cream DAC	1346001	4
D'ORODERM	Base cream DAC	1346001	1
Caelo	Base cream DAC	1387801	1
Caelo	Base cream DAC	13812013	1
Fagron	Base cream DAC	13A08-T06-000034	1
Fagron	Base cream DAC	13A09T10000232	1
Fagron	Base cream DAC	13A09-T10-232	2
Fagron	Base cream DAC	13A09-T12-236	1
Fagron	Base cream DAC	13A09-T10-000232	3
Fagron	Base cream DAC	13A09-T12-000238	1
Fagron	Base cream DAC	13A09-T14-000244	1
Fagron	Base cream DAC	13A09-T14-000244	1
Fagron	Base cream DAC	13A09-T18-000259	2
Fagron	Base cream DAC		2
Fagron	Base cream DAC	13C05-T-003297	1
Eurho/Phoenix	Base cream DAC	13C05-T03-001756	1
Fagron	Base cream DAC	13C05-T03-001756	5
Fagron	Base cream DAC	13C05-T03-001755	1
Fagron	Base cream DAC	13C05-T09-001778	3
Fagron	Base cream DAC	13C05-T06-001767	1
Fagron	Base cream DAC	13C05-T10-003297	1
Fagron	Base cream DAC	13E20-T01-003865	1
Fagron	Base cream DAC	13E21-T04-003893	1
Fagron	Base cream DAC	13E21-T05-003897	6
Phönix	Base cream DAC	13E21-T05-003897	1
Caelo	Base cream DAC	13E21-T06-003900	1
Fagron	Base cream DAC	13E21-T08-003906	9
Gehe	Base cream DAC	13E22T05003978	1
Fagron	Base cream DAC	13E22-T05-003978	1
Großhandel	Base cream DAC	13E21-T09-003911	1
Fagron	Base cream DAC	13E22-T04-003975	1
Fagron	Base cream DAC	13E23-T06-004008	3
Fagron	Base cream DAC	13E22-T07-003984	3
Fagron	Base cream DAC	13E22T09003991	1

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Supplier	Substance	Batch	Spectra
Fagron	Base cream DAC	13E23-004023	1
Fagron	Base cream DAC	13E22-T08-003987	2
Fagron	Base cream DAC	13E23-T07-004011	4
Fagron	Base cream DAC	13E23-T08-004015	1
Fagron	Base cream DAC	13E23-T09	3
Fagron	Base cream DAC	13E23-T10-004023	1
Caelo	Base cream DAC	13E23-T10-004023	2
Fagron	Base cream DAC	13h14t02006207	1
Fagron	Base cream DAC	13E23-T12	1
Fagron	Base cream DAC	13H14-T01-006202	1
Fagron	Base cream DAC	13H14T02006207	1
Caelo	Base cream DAC	13H14T05-006551	1
Maros/Phönix	Base cream DAC	13H14-To3-006212	1
Phoenix	Base cream DAC	14036001	1
Caelo	Base cream DAC	14090501	1
Caelo	Base cream DAC	1409101	1
Caelo	Base cream DAC	14121-01309	1
Caelo	Base cream DAC	14144202	1
P.W.Beyvers GmbH	Base cream DAC		3
Caelo	Base cream DAC	14A10-T06-009259	1
Hersteller: Beyvers	Base cream DAC		1
Caelo	Base cream DAC	144144201	1
p.w beyers gmbh,phönix	Base cream DAC		4
Euro OTC	Base cream DAC	150200801	1
Fagron	Base cream DAC	14D08-T03-01168	1
Caelo	Base cream DAC	14D08T04-011692	1
Euro OTC	Base cream DAC	1520202801	1
Phönix	Base cream DAC	15272601	1
Caelo	Base cream DAC	160704	1
Phönix	Base cream DAC	15450601	1
Celo	Base cream DAC	16005101	1
Caelo	Base cream DAC	16152201	1
Caelo	Base cream DAC	16135901	2
Caelo	Base cream DAC	16B290713	1
Caelo	Base cream DAC	17061305	1
Caelo	Base cream DAC	1713M-01309	1
Caelo	Base cream DAC	2025-T05	1
Caelo	Base cream DAC	19021304	1
Caelo	Base cream DAC	19101302	2
Gehe	Base cream DAC	207/1	4
P.W.Beyvers GmbH	Base cream DAC	207/1	2
Caelo	Base cream DAC	18071302	1
Fagron	Base cream DAC	16C14T03-031205	1
Gehe	Base cream DAC	207/2	1
Anzag	Base cream DAC	207/2	1
Ferdi	Base cream DAC	21220113	1
P.W.Beyvers GmbH,Phönix	Base cream DAC	207/2	1
Gehe	Base cream DAC	219/1	3
P.W.Beyvers GmbH	Base cream DAC	219/1	1
P.W. Beyvers	Base cream DAC	219/1	2
PHOENIX am 04.06.2012	Base cream DAC	219/1	3
Gehe	Base cream DAC	219/2	3
P.W.Beyvers GmbH	Base cream DAC	219/2	1
Caelo	Base cream DAC	22041306	1
Caelo	Base cream DAC	219/2	2
P.W. Beyvers	Base cream DAC	229/1	1
P.W.Beyvers GmbH	Base cream DAC	229/1	1
P.W.Beyvers	Base cream DAC	229/1	1
Caelo	Base cream DAC	2213V01309	1
P.W.Beyvers	Base cream DAC	229/1	2

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Supplier	Substance	Batch	Spectra
Caelo	Base cream DAC	22031303	1
Gehe	Base cream DAC	229/2	4
P.W.Beyvers GmbH	Base cream DAC	229/2	3
anzag, 05.11.2012	Base cream DAC	229/2	1
P.W.Beyvers	Base cream DAC	229/2	1
P.W.Beyvers	Base cream DAC	234/1	1
P.W. Beyvers	Base cream DAC	234/1	1
Beyvers	Base cream DAC	234/2	1
Gehe	Base cream DAC	234/1	1
P.W.Beyvers GmbH / Phoe...	Base cream DAC	234/1	1
Gehe 17.01.13	Base cream DAC	234/2	1
Gehe	Base cream DAC	234/2	4
P.W. Beyvers	Base cream DAC	234/3	2
P.W. Beyvers	Base cream DAC	234/2	1
P.W.Beyvers GmbH,Phönix	Base cream DAC	234/3	2
Beyvers	Base cream DAC	234/3	1
Caelo	Base cream DAC	24091301	1
Caelo	Base cream DAC	25021402	1
Ensbona/Eimermacher	Base cream DAC	24550213	1
Caelo	Base cream DAC	25011401	1
P.W.Beyvers GmbH / Phoe...	Base cream DAC	243/3	1
Caelo	Base cream DAC	26061204	1
Bombastus	Base cream DAC	272369	2
Gehe	Base cream DAC	272367	1
Gehe	Base cream DAC	272371	1
Gehe	Base cream DAC	272373	1
Bombastus	Base cream DAC	272373	1
Bombastus	Base cream DAC	272375	1
Gehe	Base cream DAC	275147	1
Bombastus	Base cream DAC	275173	1
Bombastus	Base cream DAC	275181	2
Bombastus	Base cream DAC	275184	2
Bombastus	Base cream DAC	275182	1
Bombastus	Base cream DAC	275280	1
Bombastus	Base cream DAC	275438	6
Bombastus	Base cream DAC	275273	1
Bombastus	Base cream DAC	275277	1
Bombastus	Base cream DAC	275282	1
Bombastus	Base cream DAC	275279	1
Caelo	Base cream DAC	275438	2
Bombastus	Base cream DAC	275443	1
Bombastus	Base cream DAC	275440	1
AHD, 05.04.2013	Base cream DAC	275439	1
Anzag 19.02.2013	Base cream DAC	275444	1
Bombastus	Base cream DAC	275445	1
Bombastus	Base cream DAC	275591	1
Bombastus	Base cream DAC	275447	1
Bombastus	Base cream DAC	275590	2
Phoenix	Base cream DAC	275591	1
Caelo	Base cream DAC	275591	1
Bombastus	Base cream DAC	276944	2
Bombastus	Base cream DAC	276948	1
Bombastus	Base cream DAC	276950	1
Bombastus	Base cream DAC	277099	14
phönix	Base cream DAC	277099	1
Bombastus	Base cream DAC	278396	2
Gehe	Base cream DAC	278392	2
Caelo	Base cream DAC	277111	1
Bombastus	Base cream DAC	277112	1
Bombastus	Base cream DAC	277248	1

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Supplier	Substance	Batch	Spectra
Gehe	Base cream DAC	277109	1
Gehe	Base cream DAC	278401	1
Apomix / 11	Base cream DAC	278472	2
Bombastus	Base cream DAC	278470	1
Bombastus	Base cream DAC	278397	1
Bombastus	Base cream DAC	278474	6
Bombastus	Base cream DAC	278475	1
Bombastus	Base cream DAC	278478	1
Bombastus	Base cream DAC	278553	1
Bombastus	Base cream DAC	278479	2
Phönix	Base cream DAC	278475	1
Bombastus	Base cream DAC	278476	1
Bombastus	Base cream DAC	278555	3
Bombastus	Base cream DAC	278556	6
Bombastus	Base cream DAC	278558	1
Bombastus	Base cream DAC	278559	1
Bombastus	Base cream DAC	278557	2
Bombastus	Base cream DAC	278560	2
Bombastus	Base cream DAC	278561	1
Bombastus	Base cream DAC	278562	2
Bombastus	Base cream DAC	279960	1
Bombastus	Base cream DAC	279958	3
Bombastus	Base cream DAC	279961	1
Caelo	Base cream DAC	279963	1
Phönix, 28.10.2013	Base cream DAC	279961	1
Bombastus	Base cream DAC	279964	3
Bombastus	Base cream DAC	280077	1
Taoasis	Base cream DAC	280079	2
Bombastus	Base cream DAC	280080	4
AHD, 02.12.13	Base cream DAC	280079	1
Gehe	Base cream DAC	280082	1
Caelo	Base cream DAC	28031403	1
Caelo	Base cream DAC	28031404	1
Caelo	Base cream DAC	28031401	1
gehe	Base cream DAC	281235	1
Gehe	Base cream DAC	281237	1
Bombastus	Base cream DAC	281239	1
Bombastus	Base cream DAC	281240	1
Bombastus	Base cream DAC	281328	2
Apomix / AHD	Base cream DAC	281328006/14	1
Bombastus	Base cream DAC	281331	4
Bombastus	Base cream DAC	281486	3
Bombastus	Base cream DAC	281329	1
Bombastus	Base cream DAC	282723	2
Bombastus	Base cream DAC	281332	1
Bombastus	Base cream DAC	281335	1
Bombastus	Base cream DAC	282771	1
Eimermacher	Base cream DAC	28310913	2
Bombastus	Base cream DAC	282778	1
Gehe	Base cream DAC	283975	1
Bombastus	Base cream DAC	286086	2
Caelo	Base cream DAC	2901311309	1
Bombastus	Base cream DAC	283917	1
Bombastus	Base cream DAC	299325	1
Caelo	Base cream DAC	30111201	1
Caelo	Base cream DAC	3013M-01309	1
P.W.Beyvers	Base cream DAC		1
Noweda	Base cream DAC	30241211	4
P.W. Beyvers	Base cream DAC		1
Caelo	Base cream DAC	31081205	1

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Supplier	Substance	Batch	Spectra
Beyvers	Base cream DAC		1
Gehe	Base cream DAC	319/1	2
P.W.Beyers/Phoenix	Base cream DAC	319/2	1
gehe 24.07.2013	Base cream DAC	319/1	1
P. W. Beyvers	Base cream DAC	319/1	1
P.W.Beyers/Phoenix	Base cream DAC	319/1	1
Beyvers	Base cream DAC	319/2	1
P.W. Beyvers	Base cream DAC	329/1	2
Gehe	Base cream DAC	329/1	3
P.W. Beyvers	Base cream DAC	329/2	4
P.W.Beyvers GmbH,Phönix	Base cream DAC	329/1	1
Beyvers GmbH/ Noweda	Base cream DAC	329/1	1
Gehe	Base cream DAC	329/2	1
Gehe	Base cream DAC	340/1	2
gehe 28.11.13	Base cream DAC	340/2	1
P.W.Beyvers	Base cream DAC	340/1	1
P.W.Beyvers/Jenne 18.12. ...	Base cream DAC	340/2	1
Beyvers/Gumo	Base cream DAC	340/2	1
P.W.Beyvers	Base cream DAC	340/2	3
P.W. Beyvers / Anzag	Base cream DAC	340/2	1
P.W.Beyvers GmbH/Anzag	Base cream DAC	340/2	1
Caelo	Base cream DAC	3513I-01309	1
Fagron	Base cream DAC	3613E-01309	1
Beyvers	Base cream DAC	340/2	1
Caelo	Base cream DAC	4113E-01309	1
Caelo	Base cream DAC	4121	1
P.W.Beyvers GmbH/Phönix	Base cream DAC	340/2	1
Caelo	Base cream DAC	3413E-01309	1
Eimermacher	Base cream DAC	36140913	1
anzag, 20.11.2012	Base cream DAC	412245001	1
P.W.Beyvers GmbH,Phönix	Base cream DAC	440/1	2
Caelo	Base cream DAC	4913E01309	1
Caelo	Base cream DAC	4512Q-01309	1
Caelo	Base cream DAC	5012Q-01309	1
P.W.Beyvers GmbH,Phönix	Base cream DAC	440/2	1
Noweda	Base cream DAC	5099500	3
Noweda	Base cream DAC	50995000	1
Noweda	Base cream DAC	5099900	1
Phönix Gotha	Base cream DAC	5163300	1
Henry Lamotte	Base cream DAC	5100000	1
Henry Lamotte Oils GmbH	Base cream DAC	5151700	1
Noweda	Base cream DAC	5100000	1
Henry Lamotte Oils GmbH	Base cream DAC	5163300	1
Noweda	Base cream DAC	5163300	1
Henry Lamotte Oils GmbH	Base cream DAC	5215300	3
Phönix Gotha	Base cream DAC	5215600	2
Henry Lamotte	Base cream DAC	5163400	1
Lamotte/Otto	Base cream DAC	5215800	2
Henry Lamotte	Base cream DAC	5215400	1
Henry Lamotte Oils GmbH	Base cream DAC	5215500	2
Henry Lamotte Oils GmbH	Base cream DAC	5215700	1
Henry Lamotte Oils	Base cream DAC	5215600	1
Phönix Gotha	Base cream DAC	5215800	1
Noweda	Base cream DAC	52701012	1
Ensbona/Eimermacher	Base cream DAC	52701012	1
Phoenix	Base cream DAC	5289100	1
Henry Lamotte/Anzag	Base cream DAC	5289200	1
Anzag/Henry Lamotte	Base cream DAC	5289100	1
Lamotte/Otto	Base cream DAC	5321000	1
Henry Lamotte	Base cream DAC	5289000	1

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Supplier	Substance	Batch	Spectra
Lamotte 001	Base cream DAC	5321000	1
Henry Lamotte Oils GmbH	Base cream DAC	5321000	5
Phönix Gotha	Base cream DAC	5321000	1
Anzag 11.03.13	Base cream DAC	5321100	1
Caelo	Base cream DAC	5289100	1
Henry Lamotte Oils	Base cream DAC	5321200	1
Henry Lamotte	Base cream DAC	5321100	1
Caelo	Base cream DAC	5321200	2
Noweda/Lamotte Oils	Base cream DAC	5321200	1
Phönix Gotha	Base cream DAC	5322100	1
Henry Lamotte Oils GmbH	Base cream DAC	5322100	1
Henry Lamotte Oils GmbH	Base cream DAC	5322200	1
Lamotte/Phoenix	Base cream DAC	5322200	1
Anzag 11.03.2013	Base cream DAC	5322200	1
Henry Lamotte/ Noweda	Base cream DAC	532220	1
Henry Lamotte	Base cream DAC	5322300	3
Henry Lamotte Oils	Base cream DAC	5322400	1
beyvers	Base cream DAC	538/2	2
Alliance Healthcare	Base cream DAC	5322400	1
post apotheke	Base cream DAC	540770	1
Lamotte/ Noweda	Base cream DAC	5407900	1
Henry Lamotte	Base cream DAC	5407700	1
Henry Lamotte Oils GmbH	Base cream DAC	5407700	4
Lamotte/AHD	Base cream DAC	5407900	1
lamotte	Base cream DAC	5407800	1
Henry Lamotte	Base cream DAC	5408000	1
Caelo	Base cream DAC	5408000	1
Lamotte / Anzag	Base cream DAC	5408000	1
henry Lamotte / Noweda	Base cream DAC	5408000	1
Lamotte/Anzag	Base cream DAC	5408100	1
Henry Lamotte	Base cream DAC	5408100	1
Lamotte / Anzag	Base cream DAC	5408100	1
Lamotte / Anzag	Base cream DAC	5408200	1
phönix	Base cream DAC	5408200	1
Lamotte/Anzag	Base cream DAC	5408300	2
sanacorp	Base cream DAC	548900	1
Anzag/Lamotte	Base cream DAC	5408300	1
Henry Lamotte	Base cream DAC	5408300	1
Henry Lamotte	Base cream DAC	5489800	1
Caelo	Base cream DAC	5490100	1
Henry Lamotte Oils GmbH	Base cream DAC	5490100	1
Henry Lamotte Oils GmbH...	Base cream DAC	5489900	1
Henry Lamotte Oils GmbH	Base cream DAC	5489800	1
Alliance Health 17.01.2...	Base cream DAC	5490100	1
Henry Lamotte	Base cream DAC	5490100	1
henry lamotte oils gmbh	Base cream DAC	5537000	1
Lamotte/ Noweda	Base cream DAC	5537300	1
Caelo	Base cream DAC	5490000	1
Henry Lamotte	Base cream DAC	5537100	1
Caelo	Base cream DAC	5537400	1
Henry Lamotte	Base cream DAC	6002237001	1
Henry Lamotte	Base cream DAC	6002237003	1
Henry Lamotte	Base cream DAC	5909300	1
henry lamotte	Base cream DAC	6002237003	1
Henry Lamotte Oils GmbH	Base cream DAC	6002237004	1
Bombastus	Base cream DAC	60090504	1
Bombastus	Base cream DAC	6862441	1
ensbona	Base cream DAC	74000513	1
Caelo	Base cream DAC	AKD6	1
Ensbona	Base cream DAC	98480713	1

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Supplier	Substance	Batch	Spectra
Eimermacher	Base cream DAC	97870214	2
Euro OTC	Base cream DAC	Ch1204005-01	1
Caelo	Base cream DAC	CH5490000	1
Euro OTG/ Euro OTG Pharma	Base cream DAC	1501041-01	1
P&M Cosmetics GmbH & Co...	Base cream DAC	150317	1
Caelo	Base cream DAC	15164501	1
Caelo	Base cream DAC	15391001	1
Euro OTC	Base cream DAC	1604023-01	1
Caelo	Base cream DAC	16158401	1
Caelo	Base cream DAC	1623601	1
Caelo	Base cream DAC	16232801	1
Caelo	Base cream DAC	16261701	1
Caelo	Base cream DAC	16350201	1
Lamotte/AHD	Base cream DAC	6002237009	1
Lamotte/AHD	Base cream DAC	6003682005	1
Henry Lamotte /AHD	Base cream DAC	5910000	1
henry lamotte	Base cream DAC	5537100	1
henry lamotte	Base cream DAC	5650700	1
Eimermacher Direktbezug	Base cream DAC	57080315	1
Bombastus	Base cream DAC	305729	1
Bombastus	Base cream DAC	269993	1
Lamotte/AHD	Base cream DAC	5909900	1
Bombastus	Base cream DAC	266524	1
Caelo	Base cream DAC	11279301	3
Euro OTC	Base cream DAC	1205004-01	1
Gehe	Base cream DAC	12005301	1
Dorfmeister	Base cream DAC	1205041-01	1
Anzag	Base cream DAC	1205006-01	1
Euro OTC	Base cream DAC	1212027-01	1
Euro OTC	Base cream DAC	1209039-01	1
GEHE	Base cream DAC	12174801	1
Bombastus	Base cream DAC	272372	1
Bombastus	Base cream DAC	275175	1
Gehe	Base cream DAC	275277	1
Bombastus	Base cream DAC	280082	2
Gehe	Base cream DAC	279961	1
Gehe	Base cream DAC	275590	1
Bombastus	Base cream DAC	282774	1
Anzag	Base cream DAC	5215600	1
Gehe	Base cream DAC	287941	1
Anzag	Base cream DAC	5321000	1
Fagron	Base cream DAC	5321100	1
henry lamotte	Base cream DAC	5489800	2
henry lamotte	Base cream DAC	5490100	1
Caelo	Base cream DAC	131203801	1
Gutenberg-Apotheke	Base cream DAC	13378201	1
DORODERM GmbH & Co.KG	Base cream DAC	1346001	2
Gutenberg-Apotheke	Base cream DAC	14035801	1
Caelo	Base cream DAC	14053201	1
Fagron	Base cream DAC	14223201	1
Fagron	Base cream DAC	14F05-T07-012966	1
Bombastus	Base cream DAC	287193	1
Bombastus	Base cream DAC	289591	1
Bombastus	Base cream DAC	292258	1
Bombastus	Base cream DAC	294837	1
Caelo	Base cream DAC	5537300	1
Henry Lamotte/Anzag	Base cream DAC	5651100	1
Lamotte/AHD	Base cream DAC	5651300	1
Anzah / Henry lamotte	Base cream DAC	57788600	1
Caelo	Base cream DAC	1301023-01	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Base cream DAC	13007301	1
Caelo	Base cream DAC	12344001	1
Sanacorp	Base cream DAC	13007201	1
Sanacorp	Base cream DAC	13082203	1
Fagron	Base cream DAC	13111101	1
Sanacorp	Base cream DAC	13082101	1
Sanacorp	Base cream DAC	13139801	1
Sanacorp	Base cream DAC	13158401	2
Sanacorp	Base cream DAC	13187901	1
Sanacorp	Base cream DAC	13188701	1
Sanacorp	Base cream DAC	13310901	1
Sanacorp	Base cream DAC	1317301	1
Sanacorp	Base cream DAC	13347201	1
Euro OTC	Base cream DAC	13312201	1
Caelo	Base cream DAC	13311301-3462312170	1
Fagron	Base cream DAC	13A09-T19-001952	1
Fagron	Base cream DAC	13E20-T01-003865	1
Fagron	Base cream DAC	13H14-T10-007314	1
Bombastus	Base cream DAC	282887	1

- 54 588 spectra from 331 *Apo-Ident* customers from a total of 18 652 batches from a further 328 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 *Base cream DAC* 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 *Base cream DAC* 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	590	0	33 754
Type B	0	3832	50	59 632
Type C	0	3433	420	54 582

The substance/substance group *Base cream DAC* 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 % (> 99.9689 %)	100.0000 % (> 98.9831 %)
Type B	100.0000 % (> 99.9712 %)	98.7120 % (> 98.6347 %)
Type C	100.0000 % (> 99.6016 %)	89.0994 % (> 89.0215 %)

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

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

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30923	31252	8.64	23.86
31043	31474	12.03	21.03
31252	31252	0.00	25.66
31474	31474	0.00	15.33
31709	31709	0.00	25.26
31710	31710	0.00	24.84
31711	31711	0.00	24.77
31712	31712	0.00	26.63
31713	31713	0.00	23.70
31714	31714	0.00	23.31
31715	31715	0.00	23.18
31716	31716	0.00	22.42
31964	31964	0.00	17.78
32345	31716	4.19	24.31

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Basis Cordes® RK**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30892-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Basis Cordes® RK

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Basis Cordes® RK*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Ichthyol	Basis Cordes® RK	12A114	30892	60	1405097
Ichthyol	Basis Cordes® RK	13A038	31078	40	20130301
Ichthyol	Basis Cordes® RK	14A087	31660	40	1511145

Validation samples

A total of 156 379 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 *Basis Cordes*[®] RK. These samples are listed above in the [calibration samples](#) section.
- 34 204 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 90 spectra of 3 reference samples from the substance/substance group *Basis Cordes*[®] RK.

Supplier	Substance	Batch	Sample ID	Spectra
Ichthyol	Basis Cordes [®] RK	10A001	30225	30
Ichthyol	Basis Cordes [®] RK	14A087	31660 [†]	20
Ichthyol	Basis Cordes [®] RK	16A035	32951	40

- 63 504 spectra from a total of 1474 batches from further 439 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.

- 281 spectra from 126 *Apo-Ident* customers from 46 batches from the substance/substance group *Basis Cordes*[®] RK.

Supplier	Substance	Batch	Spectra
Ichthyol	Basis Cordes [®] RK	10071401	1
Ichthyol-Gesellschaft/P...	Basis Cordes [®] RK	13A039	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
Ichthyol	Basis Cordes [®] RK	13A039	2
Ichthyol / Noweda	Basis Cordes [®] RK	13A039	3
Ichthyol-Gesellschaft/N...	Basis Cordes [®] RK	13A103	1
Ichthyol-Gesellschaft	Basis Cordes [®] RK	13A039	2
Ichthyol/Otto	Basis Cordes [®] RK	13A103	1
Ichthyol /Noweda	Basis Cordes [®] RK	13A103	3
Ichthyol/Noweda	Basis Cordes [®] RK	13A103	1
Ichthyol-Gesellschaft/G...	Basis Cordes [®] RK	13A103	2
Caelo	Basis Cordes [®] RK	13A103	1
Phönix Gotha	Basis Cordes [®] RK	13A103	2
Ichthyol/Gehe	Basis Cordes [®] RK	13A103	1
Ichthyol	Basis Cordes [®] RK	13A103	4
Ichthyol-Gesellschaft/V...	Basis Cordes [®] RK	13A103	1
Ichthyol-Gesellschaft /...	Basis Cordes [®] RK	13A103	1
Ichthyol/Alliance healt...	Basis Cordes [®] RK	13A103	1
Fagron	Basis Cordes [®] RK	13A103	2
Ichthyol/Gehe	Basis Cordes [®] RK	13A104	4
Sanacorp	Basis Cordes [®] RK	13A103	1
Ichthyol-Gesellschaft	Basis Cordes [®] RK	13A103	1
Bombastus	Basis Cordes [®] RK	13A103	1
Ichtyol/Gehe	Basis Cordes [®] RK	13A206	1
Anzag/Ichtyol-Gesellsch...	Basis Cordes [®] RK	13A104	1
Ichthyol	Basis Cordes [®] RK	13A104	4
Ichthyol-Gesellschaft/N...	Basis Cordes [®] RK	13A206	2
Caelo	Basis Cordes [®] RK	13A206	2
Ichthyol-Gesellschaft/ ...	Basis Cordes [®] RK	13A206	1
Ichthyol/Anzag	Basis Cordes [®] RK	13A206	1
Ichtyol Gehe	Basis Cordes [®] RK	13A206	1
Ichtyol-Gesellschaft	Basis Cordes [®] RK	13A206	1
Cordes, Hermani / Gehe	Basis Cordes [®] RK	13A206	1
Ichthyol-Gesellschaft	Basis Cordes [®] RK	13A206	2
Ichthyol/Sanacorp	Basis Cordes [®] RK	13A206	1
Ichtyol - Gesellschaft	Basis Cordes [®] RK	13A206	1
Ichthyol über Phoenix	Basis Cordes [®] RK	13A206	1
Ichthyol-Gesellschaft /...	Basis Cordes [®] RK	13A206	1
Ichtyol /Phönix	Basis Cordes [®] RK	13A206	1
Ichthyol/ Phoenix	Basis Cordes [®] RK	13A206	1
200	Basis Cordes [®] RK	13A206	1
Ichthyol	Basis Cordes [®] RK	13A206	2
IchthyolAlliance Health...	Basis Cordes [®] RK	13A206	1
Phönix Gotha	Basis Cordes [®] RK	13A2C6	1
Ichthyol	Basis Cordes [®] RK	14A038	1
Noweda/Ichthyol	Basis Cordes [®] RK	14A038	1
Ichthyol-Gesellschaft /...	Basis Cordes [®] RK	14A038	1
Ichthyol/Gehe	Basis Cordes [®] RK	14A038	2
Ichthyol	Basis Cordes [®] RK	14a087	1
Anzag/Ichtyol-Gesellsch...	Basis Cordes [®] RK	14A051	1
Ichtyol-Gesellschaft	Basis Cordes [®] RK	14A087	1
ICHTHYOL-GESELLSCHAFT C...	Basis Cordes [®] RK	14A087	1
Ichthyol-Gesellschaft	Basis Cordes [®] RK	14A087	2
Ichthyol /Gehe	Basis Cordes [®] RK	14A087	1
Noweda	Basis Cordes [®] RK	14A087	1
Ichthyol/Otto	Basis Cordes [®] RK	14A087	1
Ichthyol/Alliance Healt...	Basis Cordes [®] RK	14A087	1
ICHTHYOL/GEHE	Basis Cordes [®] RK	14A087	1
Ichthyol/Phoenix	Basis Cordes [®] RK	14A205	1
Ichthyol-Gesellschaft	Basis Cordes [®] RK	14A148	1
Ichthyol Gesellschaft	Basis Cordes [®] RK	14A148	1
Ichthyol-Gesellschaft	Basis Cordes [®] RK	14A205	1
Gehe/Ichthyol	Basis Cordes [®] RK	14A087	1

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Supplier	Substance	Batch	Spectra
Ichthyol/VDL	Basis Cordes® RK	14A205	1
Ichthyol-Gesellschaft	Basis Cordes® RK	14A205	2
Ichthyol / Phoenix	Basis Cordes® RK	14A205	1
Phönix Gotha	Basis Cordes® RK	14A205	1
Caelo	Basis Cordes® RK	14A205	3
Ichthyol	Basis Cordes® RK	14A205	1
Ichthyol/Noweda	Basis Cordes® RK	14A205	1
Ichthyol-Gesellschaft C...	Basis Cordes® RK	15A051	2
Phönix Gotha	Basis Cordes® RK	15A051	1
Ichthyol-Gesellschaft /...	Basis Cordes® RK	14A205	1
Caelo	Basis Cordes® RK	14D87	1
Ichthyol/Gehe	Basis Cordes® RK	14A205	1
Ichthyol/Phoenix	Basis Cordes® RK	15A057	1
Ichthyol/Anzag	Basis Cordes® RK	15A051	1
Ichthyol	Basis Cordes® RK	15A057	1
Ichthyol-Gesellschaft	Basis Cordes® RK	15A057	1
Ichthyol-Gesellschaft	Basis Cordes® RK	15A057	5
ICHTHYOL / 30	Basis Cordes® RK	15A057	1
ICHTHYOL-GESELLSCHAFT C...	Basis Cordes® RK	15A057	1
Ichthyol-Gesellschaft/A...	Basis Cordes® RK	15A057	1
Noweda	Basis Cordes® RK	15A057	1
Ichthyol	Basis Cordes® RK	15A057	2
Ichthyol / Noweda	Basis Cordes® RK	15A057	1
Ichthyol-Gesellschaft	Basis Cordes® RK	15A115	1
Caelo	Basis Cordes® RK	15A115	1
Ichthyol Gesellschaft	Basis Cordes® RK	15A115	1
Ichthyol	Basis Cordes® RK	15A115	1
Noweda 29.032016	Basis Cordes® RK	15A115	1
ICHTHYOL-GESELLSCHAFT C...	Basis Cordes® RK	15A115	1
Ichthyol/N	Basis Cordes® RK	15A115	1
Ichthyol/Noweda	Basis Cordes® RK	15a115	1
Ichthyol/Gehe	Basis Cordes® RK	15A115	2
Ichthyol Werke	Basis Cordes® RK	15A115	1
Ichthyol / Sanacorp	Basis Cordes® RK	15A115	1
Ichthyol/Sanacorp	Basis Cordes® RK	15A115	1
Caelo	Basis Cordes® RK	15A172	1
Ichthyol-Gesellschaft C...	Basis Cordes® RK	15A172	4
Ichthyol Gesellsch./Now...	Basis Cordes® RK	15A194	1
Ichthyol/Phoenix	Basis Cordes® RK	15A194	2
Ichthyol/Noweda	Basis Cordes® RK	15a194	1
Ichthyol	Basis Cordes® RK	15A172	1
Ichthyol/Sanacorp	Basis Cordes® RK	15A194	1
Noweda	Basis Cordes® RK	15A194	1
Ichthyol/Phönix	Basis Cordes® RK	15A194	1
Phönix	Basis Cordes® RK	15A194	2
Ichthyol/Alliance Healt...	Basis Cordes® RK	15A194	1
Ichthyol Werke	Basis Cordes® RK	15A194	1
ICHTHYOL / 20	Basis Cordes® RK	15A194	1
Ichthyol	Basis Cordes® RK	15A057	1
Ichthyol-Gesellschaft	Basis Cordes® RK	15A194	1
ICHTHYOL-GESELLSCHAFT	Basis Cordes® RK	16A035	1
Caelo	Basis Cordes® RK	16A035	1
Gehe/Ichthyol 23.11.16	Basis Cordes® RK	16A035	1
Ichthyol-Gesellschaft	Basis Cordes® RK	16A035	1
AHD/ichthyol	Basis Cordes® RK	16A035	1
ichthyol/noweda	Basis Cordes® RK	15A057	1
Phoe	Basis Cordes® RK	16A035	1
Ichthyol	Basis Cordes® RK	20061501	1
ICHTHYOL-GESELLSCHAFT	Basis Cordes® RK	11A079	1
Ichthyol	Basis Cordes® RK	10A064	1

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Supplier	Substance	Batch	Spectra
Caelo	Basis Cordes [®] RK	P160/14	1
Ebert	Basis Cordes [®] RK	11A079	1
Ichthyol	Basis Cordes [®] RK	28011507	1
Phönix Gotha	Basis Cordes [®] RK	11A079	1
ICHTHYOL-GES/GEHE	Basis Cordes [®] RK	11A079	1
Ichthyol Gesellschaft C...	Basis Cordes [®] RK	11A079	1
Ichthyol	Basis Cordes [®] RK	11A079	1
Ichthyol / Anzag	Basis Cordes [®] RK	11A156	1
Ichthyol	Basis Cordes [®] RK	11A156	1
Ichthyol/ Noweda	Basis Cordes [®] RK	11A079	1
Noweda	Basis Cordes [®] RK	11A156	1
Ichthyol Gesellschaft C...	Basis Cordes [®] RK	11A156	1
Ichtyol	Basis Cordes [®] RK	11A156	1
ichthyol	Basis Cordes [®] RK	1213Q-03300	1
Caelo	Basis Cordes [®] RK	12345	1
Ichthyol - Gesellschaft	Basis Cordes [®] RK	11A079	1
Ichthyol	Basis Cordes [®] RK	12A030	2
Gehe	Basis Cordes [®] RK	12A030	2
Ichthyol-Gesellschaft	Basis Cordes [®] RK	12A030	1
Ichthyol Gesellschaft C...	Basis Cordes [®] RK	12A045	1
Gehe	Basis Cordes [®] RK	12A045	4
Noweda	Basis Cordes [®] RK	12A045	1
Ichthyol-Gesellschaft C...	Basis Cordes [®] RK	12A045	1
Ichthyol-Gesellschaft / E	Basis Cordes [®] RK	12A045	1
Ichthyol Gesellschaft	Basis Cordes [®] RK	12A045	1
Sanacorp/ Ichthyol Gese...	Basis Cordes [®] RK	12A045	1
Ichthyol	Basis Cordes [®] RK	12A045	2
Phönix Gotha	Basis Cordes [®] RK	12A045	1
Ichthyol/Anzag	Basis Cordes [®] RK	12A045	1
ICHTHYOL-GES/GEHE	Basis Cordes [®] RK	12A045	1
Caelo	Basis Cordes [®] RK	12A045	1
Ichthyol/ Noweda	Basis Cordes [®] RK	12A046	1
Ichthyol-Gesellschaft	Basis Cordes [®] RK	12A046	1
Phönix/Ichthyol	Basis Cordes [®] RK	12A046	1
Noweda	Basis Cordes [®] RK	12A046	1
Ichthyol-Gesellschaft C...	Basis Cordes [®] RK	12A046	1
sanacorp	Basis Cordes [®] RK	12A046	1
Ichthyol - Gesellschaft	Basis Cordes [®] RK	12A046	1
Ichthol	Basis Cordes [®] RK	12A046	1
Anzag/Ichtyol	Basis Cordes [®] RK	12A046	1
Ichthyol	Basis Cordes [®] RK	12A046	1
Ichthyol	Basis Cordes [®] RK	12a046	1
Ichthyol Gesellschaft C...	Basis Cordes [®] RK	12A046	1
Anzag/ Ichtyol	Basis Cordes [®] RK	12A046	2
ICHTHYOL-GESELLSCHAFT	Basis Cordes [®] RK	12A046	1
ICHTHYOL-GES.	Basis Cordes [®] RK	12A114	1
Ichthyol-Gesellschaft	Basis Cordes [®] RK	12A114	1
Ichthyol	Basis Cordes [®] RK	12A114	5
Cordes/Phoenix	Basis Cordes [®] RK	12A114	1
Ichtyol	Basis Cordes [®] RK	12A114	1
Ichthyol	Basis Cordes [®] RK	12a114	1
Ichthyol Werke	Basis Cordes [®] RK	12A114	1
Ichtyol-Gesellschaft/Ph...	Basis Cordes [®] RK	12A114	1
Ichthyol/Ebert	Basis Cordes [®] RK	12A114	1
Phönix Gotha	Basis Cordes [®] RK	12A114	1
Phönix	Basis Cordes [®] RK	12A167	2
Ichthyol	Basis Cordes [®] RK	12A167	4
Ichthyol	Basis Cordes [®] RK	12a167	1
Ichthyol/N/17.04.2013/P...	Basis Cordes [®] RK	12A167	1
Sanacorp / Ichthyol	Basis Cordes [®] RK	12A167	2

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Supplier	Substance	Batch	Spectra
Cordes/Anzag	Basis Cordes [®] RK	13A038	2
Caelo	Basis Cordes [®] RK	13A038	2
Cordes/AHD	Basis Cordes [®] RK	13A038	1
Noweda	Basis Cordes [®] RK	13A038	1
Ichthyol	Basis Cordes [®] RK	13A038	6
Ichthyol , Noweda	Basis Cordes [®] RK	13A038	1
Ichthyol-Gesellschaft	Basis Cordes [®] RK	13A038	1
Ichthyol -Gesellschaft	Basis Cordes [®] RK	13A038	1
Ichthyol	Basis Cordes [®] RK	12ad30	1
Ichthyol GmbH, Phönix	Basis Cordes [®] RK	13A038	1
Ichthyol-Gesellschaft	Basis Cordes [®] RK	13A038	1
Alliance healthcare	Basis Cordes [®] RK	13A038	1
Bombastus	Basis Cordes [®] RK	13A038	1
Ichthyol-Gesellschaft / G	Basis Cordes [®] RK	13A038	1
Ichthyol, Noweda	Basis Cordes [®] RK	13A039	1
Caelo	Basis Cordes [®] RK	13A039	2
Ichthyol/gehe	Basis Cordes [®] RK	13A039	1
Gehe	Basis Cordes [®] RK	13A039	1
Ichthyol /Jenne 16.01.2014	Basis Cordes [®] RK	13A039	1
Ichthyol- Gesellschaft	Basis Cordes [®] RK	13A039	2
ichthyol/AHD	Basis Cordes [®] RK	13A039	1
Phoenix	Basis Cordes [®] RK	13A039	1
Ichthyol/gehe	Basis Cordes [®] RK	13A103	1
Ichthyol/N/PZN:01114881	Basis Cordes [®] RK	13A104	1
Ichthyol/Noweda	Basis Cordes [®] RK	13A104	1
Ichthyol Gesellschaft	Basis Cordes [®] RK	13A104	1
Ichthyol Cordes	Basis Cordes [®] RK	13A104	1
Ichthyol	Basis Cordes [®] RK	13A039	2
Ichthyol	Basis Cordes [®] RK	30041301	1
ichthyol gesellschaft	Basis Cordes [®] RK	14A205	1
Ichthyol/Gehe	Basis Cordes [®] RK	13A206	1
Caelo	Basis Cordes [®] RK	4312A-03300	1
Ichthyol	Basis Cordes [®] RK	19111208	1
Sonnenberg-Apotheke	Basis Cordes [®] RK	4643491	1

- 58 160 spectra from 332 *Apo-Ident* customers from a total of 20 047 batches from a further 328 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 *Basis Cordes[®] RK* 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 *Basis Cordes[®] RK* 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	34 204
Type B	0	90	0	63 340
Type C	0	259	22	58 065

The substance/substance group *Basis Cordes*[®] *RK* 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 % (> 99.9690 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9714 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.5979 %)	92.1708 % (> 91.1032 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30892	30892	0.00	40.64
31078	30892	5.78	45.53
31660	31660	0.00	40.03

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Benzalkonium chloride solution 50%**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30667-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Benzalkonium chloride solution 50%; Benzalkonii chloridi solutio 50%; Solutio benzalkonii chlorati 50%

Special notes

When selecting the *Benzalkonium chloride solution 50%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Benzalkonium chloride solution 50%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzalkonium chl...	11271919	30667	40	1402369
Euro OTC	Benzalkonium chl...	1105041V-03	31613	40	20130809

Validation samples

A total of 156379 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 *Benzalkonium chloride solution 50%*. These samples are listed above in the [calibration samples](#) section.
- 34264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 140 spectra of 4 reference samples from the substance/substance group *Benzalkonium chloride solution 50%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Benzalkonium chloride soluti...	112719106	30543	40
Euro OTC	Benzalkonium chloride soluti...	1105041-01	30646	40
Euro OTC	Benzalkonium chloride soluti...	1105041V-03	31613 [†]	20
Caelo	Benzalkonium chloride soluti...	15051305	32960	40

- 63454 spectra from a total of 1473 batches from further 439 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.

- 85 spectra from 56 *Apo-Ident* customers from 31 batches from the substance/substance group *Benzalkonium chloride solution 50%*.

Supplier	Substance	Batch	Spectra
Caelo	Benzalkonium chloride soluti...	8041406	1

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Benzalkonium chloride soluti...	1105041V	1
Caelo	Benzalkonium chloride soluti...	13152111	4
Caelo	Benzalkonium chloride soluti...	13152105	6
Caelo	Benzalkonium chloride soluti...	13152114	1
Caelo	Benzalkonium chloride soluti...	13152115	1
Caelo	Benzalkonium chloride soluti...	13152121	1
Caelo	Benzalkonium chloride soluti...	13152123	3
Caelo	Benzalkonium chloride soluti...	13152125	12
Gehe	Benzalkonium chloride soluti...	13152123	1
Phönix	Benzalkonium chloride soluti...	13152125	1
Sanacorp	Benzalkonium chloride soluti...	13152125	1
Caelo	Benzalkonium chloride soluti...	15051305	5
Phönix Gotha	Benzalkonium chloride soluti...	13152125	1
Phoenix	Benzalkonium chloride soluti...	15051309	1
Caelo	Benzalkonium chloride soluti...	15051317	2
Caelo	Benzalkonium chloride soluti...	15051309	2
Caelo	Benzalkonium chloride soluti...	15119501	3
Caelo	Benzalkonium chloride soluti...	15119505	5
Sanacorp	Benzalkonium chloride soluti...	4/AKD2	1
Fagron	Benzalkonium chloride soluti...	1105041-01	2
Fagron	Benzalkonium chloride soluti...	15119501	1
Caelo	Benzalkonium chloride soluti...	611benz	1
Fagron	Benzalkonium chloride soluti...	7F21-N09	1
Euro OTC	Benzalkonium chloride soluti...	1105041-01	2
Gehe	Benzalkonium chloride soluti...	1105041-01	1
Euro OTC	Benzalkonium chloride soluti...	1105041V-03	2
Caelo	Benzalkonium chloride soluti...	11271906	2
Caelo	Benzalkonium chloride soluti...	11271912	1
Caelo	Benzalkonium chloride soluti...	11271919	3
Caelo	Benzalkonium chloride soluti...	12254603	1
Sanacorp	Benzalkonium chloride soluti...	12254608	1
Caelo	Benzalkonium chloride soluti...	12254608	2
Noweda	Benzalkonium chloride soluti...	12254615	1
Caelo	Benzalkonium chloride soluti...	12254615	2
Caelo	Benzalkonium chloride soluti...	12254610	2
Caelo	Benzalkonium chloride soluti...	12254620	3
Caelo	Benzalkonium chloride soluti...	1315225	1
Fagron	Benzalkonium chloride soluti...	2913A-01168	1
Löhr Center/	Benzalkonium chloride soluti...	2013U-01168	1
Caelo	Benzalkonium chloride soluti...	31011402	1

- 58 356 spectra from 332 *Apo-Ident* customers from a total of 20 062 batches from a further 328 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 *Benzalkonium chloride solution 50%* 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 *Benzalkonium chloride solution 50%* 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	34 264
Type B	0	139	1	63 454
Type C	0	84	1	58 356

The substance/substance group *Benzalkonium chloride solution 50%* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9710 %)	99.2857 % (> 97.1429 %)
Type C	100.0000 % (> 99.5964 %)	98.8235 % (> 95.2941 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30667	30667	0.00	53.67
31613	30667	7.59	52.99

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Benzyl alcohol**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30574-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Benzyl alcohol; Alkohol benzylicus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Benzyl alcohol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzyl alcohol	13292103	31220	40	1403478
Caelo	Benzyl alcohol	13292107	31369	60	20131028

Validation samples

A total of 156 379 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 *Benzyl alcohol*. These samples are listed above in the [calibration samples](#) section.
- 34 244 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 50 spectra of 2 reference samples from the substance/substance group *Benzyl alcohol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Benzyl alcohol	12108503	30574	40
Caelo	Benzyl alcohol	13292107	31369 [†]	10

- 63 544 spectra from a total of 1475 batches from further 439 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 7 *Apo-Ident* customers from 14 batches from the substance/substance group *Benzyl alcohol*.

Supplier	Substance	Batch	Spectra
Caelo	Benzyl alcohol	13292103	3
Caelo	Benzyl alcohol	13292107	2
Caelo	Benzyl alcohol	14206201	2

continued on the next page

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

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Supplier	Substance	Batch	Spectra
Caelo	Benzyl alcohol	15014901	4
Caelo	Benzyl alcohol	14206209	1
Sanacorp	Benzyl alcohol	15014907	1
Caelo	Benzyl alcohol	15318403	2
Caelo	Benzyl alcohol	15437503	2
Gehe	Benzyl alcohol	15437503	1
Caelo	Benzyl alcohol	15014907	1
Gehe	Benzyl alcohol	15437509	1
Gehe	Benzyl alcohol	15318406	1
Caelo	Benzyl alcohol	12108503	1
Gehe	Benzyl alcohol	15437512	1
Caelo	Benzyl alcohol	12256208	1
Caelo	Benzyl alcohol	13056803	1

- 58 416 spectra from 332 *Apo-Ident* customers from a total of 20 078 batches from a further 328 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 *Benzyl alcohol* 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 *Benzyl alcohol* 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	34 244
Type B	0	50	0	63 544
Type C	0	23	2	58 416

The substance/substance group *Benzyl alcohol* 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 % (> 99.9691 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 88.0000 %)
Type C	100.0000 % (> 99.5966 %)	92.0000 % (> 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.

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
31220	31220	0.00	118.34
31369	31220	2.74	119.09

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Benzyl benzoate**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31208-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Benzyl benzoate; Benzylum benzoicum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Benzyl benzoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzyl benzoate	13099320	31208	40	1403156
Caelo	Benzyl benzoate	14029602	31435	40	20140207

Validation samples

A total of 156 379 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 *Benzyl benzoate*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Benzyl benzoate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Benzyl benzoate	9362308	30320	40
Caelo	Benzyl benzoate	14029602	31435 [†]	20

- 63 534 spectra from a total of 1475 batches from further 439 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 6 *Apo-Ident* customers from 10 batches from the substance/substance group *Benzyl benzoate*.

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Benzyl benzoate	13099313	1
Caesar & Loretz GmbH	Benzyl benzoate	14029613	1
Caesar & Loretz GmbH	Benzyl benzoate	14029603	1

continued on the next page

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

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Supplier	Substance	Batch	Spectra
Caelo	Benzyl benzoate	15133401	1
Caelo	Benzyl benzoate	15243005	1
Caesar & Loretz GmbH	Benzyl benzoate	15133401	1
Bombastus	Benzyl benzoate	16140807	1
Caelo	Benzyl benzoate	11340415	1
Caesar & Loretz GmbH	Benzyl benzoate	12141003	2
Gehe	Benzyl benzoate	13099317	1
Phönix	Benzyl benzoate	12141008	1
Caelo	Benzyl benzoate	14029613	1

- 58 428 spectra from 332 *Apo-Ident* customers from a total of 20 082 batches from a further 328 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 *Benzyl benzoate* 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 *Benzyl benzoate* 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	34 264
Type B	0	55	5	63 534
Type C	0	12	1	58 428

The substance/substance group *Benzyl benzoate* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	91.6667 % (> 86.6667 %)
Type C	100.0000 % (> 99.5970 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31208	31208	0.00	49.37
31435	31208	2.07	52.19

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Benzyl nicotinate**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30502-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Benzyl nicotinate; Benzyliis nicotinas; Benzylum nicotinicum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Benzyl nicotinate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzyl nicotinate	13272502	31199	40	1403109
Caelo	Benzyl nicotinate	14112404	31383	40	20140407
Caelo	Benzyl nicotinate	163583	33055	40	20170113*

Validation samples

A total of 156 379 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 *Benzyl nicotinate*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

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

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Benzyl nicotinate	12D25-N07	30502	40
Caelo	Benzyl nicotinate	11358501	30527	40
Caelo	Benzyl nicotinate	11358505	30528	40
Caelo	Benzyl nicotinate	15444804	32592	40

- 63 434 spectra from a total of 1473 batches from further 439 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 22 *Apo-Ident* customers from 19 batches from the substance/substance group *Benzyl nicotinate*.

Supplier	Substance	Batch	Spectra
Beiersdorf AG	Benzyl nicotinate	15293104	1

continued on the next page

*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	Spectra
Anzag	Benzyl nicotinate	12282802	1
Caelo	Benzyl nicotinate	13157201	1
Caelo	Benzyl nicotinate	12142008	2
Caelo	Benzyl nicotinate	10111403	1
Caelo	Benzyl nicotinate	14112404	1
Caelo	Benzyl nicotinate	13272502	2
Caelo	Benzyl nicotinate	14112408	4
Caelo	Benzyl nicotinate	15124402	4
Caelo	Benzyl nicotinate	2091301	1
Caelo	Benzyl nicotinate	12282802	2
Caelo	Benzyl nicotinate	15124408	1
Caelo	Benzyl nicotinate	12142004	1
Caelo	Benzyl nicotinate	1529304	1
Anzag 10.08.2012	Benzyl nicotinate	12142004	1
Caelo	Benzyl nicotinate	12282804	1
VDL	Benzyl nicotinate	12D25-N07	1
Fagron	Benzyl nicotinate	12I20-N01	1
Caelo	Benzyl nicotinate	13035402	2
anzag	Benzyl nicotinate	12282802	1
Caelo	Benzyl nicotinate	13157205	3
Anzag/ichthyol	Benzyl nicotinate	13035408	1
Phönix 28.01.2014	Benzyl nicotinate	13272502	1

- 58 406 spectra from 332 *Apo-Ident* customers from a total of 20 073 batches from a further 328 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 *Benzyl nicotinate* 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 *Benzyl nicotinate* 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	34 224
Type B	0	160	0	63 434
Type C	0	33	2	58 406

The substance/substance group *Benzyl nicotinate* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.5965 %)	94.2857 % (> 85.7143 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31199	31199	0.00	32.23
31383	31199	3.30	30.03
33055	33055	0.00	33.95

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Bergamot oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31678-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bergamot oil; Oleum bergamottae; Oleum citrus bergamia

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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
Caelo	Bergamot oil	15042001	31678	40	AR-15-FG-008850-02
Caelo	Bergamot oil	15042001	31696	40	20150217

Validation samples

A total of 156 379 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 *Bergamot oil*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 797 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 52 spectra of 3 reference samples from the substance/substance group *Bergamot oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Bergamot oil	15042001	31678 [†]	20
Caelo	Bergamot oil	15042001	31696 [†]	20
Caelo	Bergamot oil	16083601	not required	12

- 63 542 spectra from a total of 1475 batches from further 439 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 *Bergamot oil*.

Supplier	Substance	Batch	Spectra
Taoasis	Bergamot oil	19821-122171	1
Caelo	Bergamot oil	15042001	1

[†]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*.

- 58 439 spectra from 332 *Apo-Ident* customers from a total of 20 090 batches from a further 328 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	80	0	34 264
Type B	0	52	0	63 542
Type C	0	2	0	58 439

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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 88.4615 %)
Type C	100.0000 % (> 99.6008 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31678	31678	0.00	61.78
31696	31678	1.33	62.76

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Cajeput
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31502-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cajeput; Oleum Cajeputi artificiale

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cajeput	13141409	31502	40	1412341
Caelo	Cajeput	14225206	31605	40	20140730

Validation samples

A total of 156 379 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 *Cajeput*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 3 reference samples from the substance/substance group *Cajeput*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cajeput	13141409	31502 [†]	20
Caelo	Cajeput	14225206	31605 [†]	20
Caelo	Cajeput	162770	32688	40

- 63 514 spectra from a total of 1474 batches from further 439 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 4 batches from the substance/substance group *Cajeput*.

Supplier	Substance	Batch	Spectra
Taoasis	Cajeput	6781010-120111	1
Taoasis	Cajeput	1518-122595	1

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz/Noweda	Cajeput	14225210	1
Taoasis	Cajeput	6781012-119058	1

- 58 437 spectra from 332 *Apo-Ident* customers from a total of 20 088 batches from a further 328 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* 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* 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	34 264
Type B	0	80	0	63 514
Type C	0	3	1	58 437

The substance/substance group *Cajeput* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5985 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31502	31502	0.00	21.17
31605	31502	11.18	19.34

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Campher spirit
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30937-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Campher spirit; Spiritus camphoratus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Campher spirit*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Campher spirit	12196804	30937	50	20120721
Caelo	Campher spirit	13354201	31389	40	1506005
Euro OTC	Campher spirit	1506006	31700	40	20150625*
Euro OTC	Campher spirit	1506007	31701	40	20150625*
Caelo	Campher spirit	16039501	32307	40	20160229

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 210 spectra of 5 reference samples from the substance/substance group *Campher spirit*. These samples are listed above in the [calibration samples](#) section.
- 34 134 spectra from a total of 793 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 3 reference samples from the substance/substance group *Campher spirit*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Campher spirit	10058403	30410	40
Euro OTC	Campher spirit	1506006	31700 [†]	20
Euro OTC	Campher spirit	1506007	31701 [†]	20

- 63 514 spectra from a total of 1474 batches from further 439 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.

- 60 spectra from 39 *Apo-Ident* customers from 32 batches from the substance/substance group *Campher spirit*.

*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.

[†]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*.

Supplier	Substance	Batch	Spectra
Euro OTC	Campher spirit	1307040	1
Caelo	Campher spirit	5031507	1
Caelo	Campher spirit	13354204	2
Caelo	Campher spirit	13354206	1
GEHE	Campher spirit	1301024-02	1
Caelo	Campher spirit	13354210	1
Euro OTC	Campher spirit	1405029-01	4
Euro OTC	Campher spirit	1405030	1
Euro OTC	Campher spirit	1405026-01	1
Euro OTC	Campher spirit	1405030-01	2
Caelo	Campher spirit	16039505	2
Euro OTC	Campher spirit	140503010	1
Caelo	Campher spirit	16039501	1
Caelo	Campher spirit		1
Caelo	Campher spirit	10058403	2
Caelo	Campher spirit	16141105	1
Euro OTC	Campher spirit	110022-02	1
Caelo	Campher spirit	11347401	3
Euro OTC	Campher spirit	1108022-02	1
Euro OTC	Campher spirit	1210028-01	5
Anzag ek:13.14EUR 14.08.12	Campher spirit	11347401	1
anzag, 05.12.2012	Campher spirit	11347401	1
ANZAG	Campher spirit	121002801	1
Euro OTC	Campher spirit	121028-01	1
Caelo	Campher spirit	12196803	6
Caelo	Campher spirit	12196804	1
Spreewälder/AHD	Campher spirit	1301024-02	1
Euro OTC	Campher spirit	1307039-01	4
Phoenix 03.12.12	Campher spirit	1307039-01	1
Euro OTC	Campher spirit	1301024-02	2
Euro OTC	Campher spirit	1307040-01	1
Euro OTC	Campher spirit	19071208	1
Caelo	Campher spirit	30101309	1
Caelo	Campher spirit	22101201	1
Caelo	Campher spirit	140503001	1
Caelo	Campher spirit	62143436	1
Euro OTC	Campher spirit	1108022-01	1
Caleo/ Anzag	Campher spirit	11347401	1

- 58 381 spectra from 332 *Apo-Ident* customers from a total of 20 061 batches from a further 328 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 *Campher spirit* 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 *Campher spirit* 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	210	0	34 134
Type B	0	80	0	63 514
Type C	0	59	1	58 381

The substance/substance group *Campher spirit* 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 % (> 99.9690 %)	100.0000 % (> 97.1429 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5964 %)	98.3333 % (> 93.3333 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30937	31389	5.67	91.44
31389	31389	0.00	97.45
31700	31700	0.00	93.30
31701	31701	0.00	95.66
32307	31389	5.78	97.26

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Camphor oil 20%**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30551-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Camphor oil 20%; Oleum camphoratum 20 %; Oleum camphoratum 20%

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 20%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Camphor oil 20%	12261202	31154	40	1404534
Caelo	Camphor oil 20%	13369902	31347	40	20131112

Validation samples

A total of 156 379 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 20%*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Camphor oil 20%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Camphor oil 20%	11121003	30551	40
Caelo	Camphor oil 20%	13369902	31347 [†]	20

- 63 534 spectra from a total of 1475 batches from further 439 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.

- 33 spectra from 16 *Apo-Ident* customers from 13 batches from the substance/substance group *Camphor oil 20%*.

Supplier	Substance	Batch	Spectra
Caelo	Camphor oil 20%	15246809	3
Noweda	Camphor oil 20%	14147303	1
Caelo	Camphor oil 20%	9250001	3

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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
Caelo	Camphor oil 20%	13369902	2
ahd/lamotte	Camphor oil 20%	133699902	1
Caelo	Camphor oil 20%	14028202	2
Caelo	Camphor oil 20%	15056906	1
Caelo	Camphor oil 20%	15056907	5
Caelo	Camphor oil 20%	16085301	1
Caelo	Camphor oil 20%	12122502	7
Caelo	Camphor oil 20%	12261203	2
Caelo	Camphor oil 20%	13039603	1
Phönix	Camphor oil 20%	13039603	1
Sanacorp	Camphor oil 20%	13039603	1
Caelo	Camphor oil 20%	1226103	1
Caelo	Camphor oil 20%	14147303	1

- 58 408 spectra from 332 *Apo-Ident* customers from a total of 20 079 batches from a further 328 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 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 *Camphor 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	80	0	34 264
Type B	0	60	0	63 534
Type C	0	32	1	58 408

The substance/substance group *Camphor 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.5966 %)	96.9697 % (> 87.8788 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31154	31154	0.00	28.94
31347	31154	2.18	28.40

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Caraway oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30876-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Caraway oil; Carvi aetheroleum; Oleum carvi

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Caraway oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Caraway oil	12J22-N03	30876	39	20121025
Caelo	Caraway oil	12043508	31024	40	AR-14-FG-012307-01
Caelo	Caraway oil	14166811	31666	40	20140604

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 119 spectra of 3 reference samples from the substance/substance group *Caraway oil*. These samples are listed above in the [calibration samples](#) section.
- 34 225 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Caraway oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Caraway oil	14166811	31666 [†]	20
Caelo	Caraway oil	16252906	33252	40

- 63 534 spectra from a total of 1475 batches from further 439 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.

- 115 spectra from 57 *Apo-Ident* customers from 60 batches from the substance/substance group *Caraway oil*.

Supplier	Substance	Batch	Spectra
Bombastus	Caraway oil	280523	1
Caelo	Caraway oil	14166803	2
Caesar/Noweda	Caraway oil	712Q-01968	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
Caelo	Caraway oil	5091402	1
Caelo	Caraway oil	6091401	1
Caelo	Caraway oil	10319117	1
Caelo	Caraway oil	10319116	1
Caelo	Caraway oil	10319115	2
Caelo	Caraway oil	2031504	1
Caelo	Caraway oil	10319108	1
Noweda	Caraway oil	10319109	1
Caelo	Caraway oil	10319118	5
Caelo	Caraway oil	10319120	2
Fagron	Caraway oil	11/13-N03	2
Schubert	Caraway oil	1031E0-801	1
Großhandel	Caraway oil	11L13N03	1
Fagron	Caraway oil	11A19-N08	1
Fagron	Caraway oil	11L13-N03	2
Caelo	Caraway oil	12043502	2
Caelo	Caraway oil	12013508	1
Caelo	Caraway oil	12043503	4
Caelo	Caraway oil	12043507	3
Caelo	Caraway oil	12043508	3
Caelo	Caraway oil	12043511	9
Phönix	Caraway oil	12043511	1
Caelo	Caraway oil	12043512	1
Fagron	Caraway oil	12J22-N03	1
Caelo	Caraway oil	12043513	7
Phönix	Caraway oil	12J22-N03	1
Fagron	Caraway oil	13c08-N03	1
Fagron	Caraway oil	12J2-N03	1
Fagron	Caraway oil	13C08-N03	3
Fagron	Caraway oil	13c08-N08	1
Großhandel	Caraway oil	13E06-N13	1
Fagron	Caraway oil	13E06-N13	3
Caelo	Caraway oil	14166812	1
Caelo	Caraway oil	14166802	3
Caelo	Caraway oil	15085704	2
Caelo	Caraway oil	14166806	1
Caelo	Caraway oil	14166811	1
Caelo	Caraway oil	15085707	4
Caelo	Caraway oil	15085709	2
Bombastus	Caraway oil	268955	1
Caelo	Caraway oil	22051306	1
Caelo	Caraway oil	19121207	1
Anzag 16.06.2010	Caraway oil	2410Q-01968	1
Caelo	Caraway oil	17101301	1
Bombastus	Caraway oil	274361	2
Caelo	Caraway oil	15085710	1
Bombastus	Caraway oil	270424	2
Klenk	Caraway oil	274361	1
Caelo	Caraway oil	27041503	1
Bombastus	Caraway oil	276856	2
Phönix	Caraway oil	276856	1
phönix 14.08.2013	Caraway oil	276856	1
Caelo	Caraway oil	28091205	1
Bombastus	Caraway oil	297505	2
Bombastus	Caraway oil	284758	2
Bombastus	Caraway oil	289019	1
Bombastus	Caraway oil	290759	1
Bombastus	Caraway oil	287725	1
Bombastus	Caraway oil	291934	3
Fagron	Caraway oil	628194	1

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Supplier	Substance	Batch	Spectra
	Caraway oil	81816288	1
Fagron	Caraway oil	699440	1
Bombastus	Caraway oil	287889	1

- 58 326 spectra from 332 *Apo-Ident* customers from a total of 20 032 batches from a further 328 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 *Caraway 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 *Caraway 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	119	0	34 225
Type B	0	60	0	63 534
Type C	0	111	4	58 326

The substance/substance group *Caraway 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 % (> 99.9691 %)	100.0000 % (> 94.9580 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.5964 %)	96.5217 % (> 93.9130 %)

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.

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
30876	31024	7.52	32.33
31024	31024	0.00	35.59
31666	31024	11.55	33.28

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Castor oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30432-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Castor oil; Oleum ricini; Ricini oleum

Special notes

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

- Advice for the identification of castor oil or rizol raw material: Castor oil and rizol (castor oil enriched with oxygen) can not be conclusively distinguished by spectral analysis. An additional analysis of identity may be required.

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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 *Castor oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Castor oil	12114603	30741	40	20120504
Caelo	Castor oil	14020104	31343	40	AR-15-FG-005211-01
Euro OTC	Castor oil	1509003	31739	45	20150918*
Caelo	Castor oil	14304807	31751	40	20141106

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Castor oil	15D02-B02-314240	31824	40	20150410
Euro OTC	Castor oil	1512024	31845	40	20160111*
Fagron	Castor oil	16J12-B01-328159	32943	40	20161121

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 285 spectra of 7 reference samples from the substance/substance group *Castor oil*. These samples are listed above in the [calibration samples](#) section.
- 34 059 spectra from a total of 791 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 635 spectra of 18 reference samples from the substance/substance group *Castor oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Bombastus	Castor oil	266593	30432	40
Euro OTC	Castor oil	1109001-01	30608	40
Caelo	Castor oil	12149306	30776	40
Euro OTC	Castor oil	1509003	31739 [†]	15
Caelo	Castor oil	14304807	31751 [†]	20
Fagron	Castor oil	15D02-B02-314240	31824 [†]	20
Euro OTC	Castor oil	1512024	31845 [†]	20
Euro OTC	Castor oil	1604019	32192	40
Caelo	Castor oil	161028	32201	40
Caelo	Castor oil	160922	32207	40
Caelo	Castor oil	162000	32311	40
Caelo	Castor oil	161672	32312	40
Caelo	Castor oil	162362	32344	40
Caelo	Castor oil	162731	32681	40
Euro OTC	Castor oil	1611005	32858	40
Caelo	Castor oil	170272	33071	40
Caelo	Castor oil	163146	33072	40
Caelo	Castor oil	170271	33073	40

*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.

- 62 959 spectra from a total of 1459 batches from further 439 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.

- 991 spectra from 208 *Apo-Ident* customers from 231 batches from the substance/substance group *Castor oil*.

Supplier	Substance	Batch	Spectra
Caelo	Castor oil	11359502	1
Euro OTC	Castor oil	121008-01	1
Phönix	Castor oil	1212008-01	1
GEHE	Castor oil	11359507	1
Caelo	Castor oil	12114605	11
Caelo	Castor oil	12114603	2
Caelo	Castor oil	12114606	2
Euro OTC	Castor oil	1212008-01	4
Euro OTC	Castor oil	1212008-02	6
Caelo	Castor oil	12270106	8
Caelo	Castor oil	12270108	3
Fagron	Castor oil	12H29-N04	2
EuRho	Castor oil	1304013-01	1
Euro OTC	Castor oil	1304013-02	10
Euro OTC	Castor oil	1304013-01	8
Caelo	Castor oil	13096304	8
Euro OTC	Castor oil	1308019-01	10
Caelo	Castor oil	13134604	22
Caelo	Castor oil	13134609	13
Fagron	Castor oil	13C08-N08	2
gehe 25.07.2013	Castor oil	275937	1
Caelo	Castor oil	278661	4
Euro OTC	Castor oil	3413U03553	1
Fargon /12.07.2013 / No...	Castor oil	13D29-N01	1
Euro OTC	Castor oil	1407053-01	3
Henry Lamotte oils GmbH...	Castor oil	10000000714	1
Euro OTC	Castor oil	1412006-02	7
Caelo	Castor oil	14144305	1
Euro OTC	Castor oil	1412006-01	5
Caelo	Castor oil	14199603	3
Euro OTC	Castor oil	1509003-01	13
Caelo	Castor oil	1504006-02	1
Euro OTC	Castor oil	1512024-02	6
Caelo	Castor oil	15392001	5
Euro OTC	Castor oil	1509003-02	8
Caelo	Castor oil	16016206	3
Caelo	Castor oil	15144304	3
Caelo	Castor oil	16016207	1
Euro OTC	Castor oil	1604019-01	10

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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
HenryLamotte/Anzag	Castor oil	2114I-02009	1
Bombastus	Castor oil	294668	8
Bombastus	Castor oil	290212	3
Caelo	Castor oil	290212	3
Bombastus	Castor oil	292409	12
Bombastus	Castor oil	295412	9
Bombastus	Castor oil	296751	7
Bombastus	Castor oil	300629	8
Bombastus	Castor oil	298699	11
Caelo	Castor oil	12270111	4
Jenne,Lamotte	Castor oil	123384	1
Anzag	Castor oil	5334001	4
Caelo	Castor oil	13043601	12
Bombastus	Castor oil	273390	5
Bombastus	Castor oil	270580	1
Phönix	Castor oil	123384	1
Noweda / Henry Lamotte	Castor oil	123384	2
Lamotte / Gehe	Castor oil	123384	2
Lamotte	Castor oil	123812	2
Otto Fischar	Castor oil	1000001914	1
Caelo	Castor oil	12318204	1
Lamotte/Anzag	Castor oil	123384L902	1
Euro OTC	Castor oil	1206039-01	4
Caelo	Castor oil	12149306	7
Caelo	Castor oil	12121307	1
Phönix	Castor oil	13043601	1
Caelo	Castor oil	13065405	24
Caelo	Castor oil	22071302	1
Caelo	Castor oil	22051303	1
Bombastus	Castor oil	275937	10
Bombastus	Castor oil	273882	8
Bombastus	Castor oil	275938	12
Anzag 15.03.2013	Castor oil	275938	1
Bombastu-Werke AG/Gehe	Castor oil	278660	1
Anzag 06.05.2013	Castor oil	278661	2
Bombastus	Castor oil	278661	11
Noweda / Henry Lamotte	Castor oil	5334001	2
Caelo	Castor oil	5334001	1
Bombastus	Castor oil	280791	16
Bombastus	Castor oil	281943	14
Caelo	Castor oil	30031302	1
Lamotte / Gehe	Castor oil	5334001	1
phö	Castor oil	5450801	1
Henry Lamotte Oils/Gehe	Castor oil	5334001	2
Lamotte	Castor oil	5450801	4
Henry Lamotte/Ebert	Castor oil	5450801	3
Caelo	Castor oil	5450801	4
Henry Lamotte	Castor oil	5450801	1
Euro OTC	Castor oil	1403024-01	6
Caelo	Castor oil	13196309	8
Caelo	Castor oil	14058810	5
Gutenberg-Apotheke	Castor oil	281944	2
Caelo	Castor oil	14199501	8
Bombastus	Castor oil	281944	6
Bombastus	Castor oil	291722	10
Caelo	Castor oil	14199502	3
Caelo	Castor oil	P161/14	1
Caelo	Castor oil	13134603-3417310103	1
Fagron	Castor oil	13134609	1
Caelo	Castor oil	13134608-3438311151	1

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Supplier	Substance	Batch	Spectra
Caelo	Castor oil	13196313	13
Caelo	Castor oil	13G29-B01	1
Lamotte/N/04.06.13/PZN:...	Castor oil	123384	1
Lamotte Phönix	Castor oil	5450801	2
Sanacorp	Castor oil	12270111	1
Henry Lamotte / Noweda	Castor oil	123384	1
Caelo	Castor oil	123384	2
Noweda/Henry Lamotte	Castor oil	123812	4
Henry Lamotte Oils GmbH...	Castor oil	123384	1
Caelo	Castor oil	1091505	1
Phoenix/Lamotte	Castor oil	123812	2
Sanacorp	Castor oil	123812	3
Henry Lamotte Oils/Noweda	Castor oil	123812	1
Henry Lamotte	Castor oil	123812	1
Lamotte/Gehe	Castor oil	123812	2
H.Lamotte/Noweda	Castor oil	123812	1
Lamotte/Anzag	Castor oil	123812	1
Stumpf/Henry Lamotte	Castor oil	124189	4
Henry Lamotte/Noweda	Castor oil	123812	1
Caelo	Castor oil	124189	2
Henry Lamotte Oils GmbH	Castor oil	123812	1
Lamotte/Sanacorp	Castor oil	124189	2
Henry Lamotte Oils GmbH...	Castor oil	124189	1
Lamotte	Castor oil	124189	2
lamotte/Gehe	Castor oil	124189	2
Henry Lamotte/Sanacorp	Castor oil	124189	1
Lamotte/Phoenix	Castor oil	124189	1
lamotte/Gehe	Castor oil	124637	1
Caelo	Castor oil	124637	1
Henry Lamotte Oils GmbH.	Castor oil	124189	1
Henry Lamotte Oils/GEHE	Castor oil	124637	1
Henry Lamotte/Noweda	Castor oil	124637	1
Stumpf/Henry Lamotte	Castor oil	125162	1
Hedinger	Castor oil	125162	1
Caelo	Castor oil	6051411	1
Lamotte / Noweda	Castor oil	125162	1
lamotte phönix	Castor oil	125162	1
Bombastus	Castor oil	415Q-02009	1
Noweda/Henry Lamotte	Castor oil	125473	1
gehe	Castor oil	6861795	1
Henry Lamotte / Kehr	Castor oil	1000000714	1
Henry Lamotte/AHD	Castor oil	1000001128	2
Henry Lamotte Oils GmbH	Castor oil	1000000714	1
Noweda/Henry Lamotte	Castor oil	1000001914	1
Henry Lamotte oils GmbH...	Castor oil	1000001128	1
Henry Lamotte/Gehe	Castor oil	1000001128	1
Lamotte/Anzag	Castor oil	1000002384	1
Henry Lamotte/Noweda	Castor oil	1000001914	1
Caelo	Castor oil	1000003564	1
Henry Lamotte/ Phönix	Castor oil	1000003564	1
Caelo	Castor oil	1000002384	1
Caelo	Castor oil	10021402	1
Henry Lamotte/Noweda	Castor oil	1000002384	1
Henry Lamotte/ Phönix	Castor oil	1000004198	1
Euro OTC	Castor oil	1014A03553	1
Bombastus	Castor oil	110816-3	1
EuRho	Castor oil	1206039-02	1
EuRho/Phönix	Castor oil	1212008-01	1
Lamotte/gehe	Castor oil	125162	1
Lamotte/gehe	Castor oil	1241892	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Castor oil	130260	1
Fagron	Castor oil	127170	1
Euro OTC	Castor oil	128224	1
Sanacorp	Castor oil	128224	1
Eurho	Castor oil	1304013-01	1
Fagron	Castor oil	13/27-B01-287857	1
Großhandel	Castor oil	1304013-01	1
EuRho/Geilenkirchen	Castor oil	1304013-02	1
EuRho	Castor oil	1304013-02	1
Großhandel	Castor oil	1304013-02	1
Euro OTC	Castor oil	130401302	1
Euro OTC	Castor oil	130401313-02	1
Caelo	Castor oil	13065401	1
Fagron	Castor oil	13065405	1
Euro OTC	Castor oil	13071301	2
EuRho/Noweda	Castor oil	1308019-01	2
Phönix	Castor oil	1308019-01	1
Euro OTC	Castor oil	130801902	1
Großhandel	Castor oil	1308019-02	1
Euro OTC	Castor oil	1308019-02	2
Caelo	Castor oil	1308019-02	1
Caelo	Castor oil	13134603	3
Caelo	Castor oil	131344604	1
Caelo	Castor oil	13134608	6
Caelo	Castor oil	13174507	1
Sanacorp	Castor oil	13196308	1
Caelo	Castor oil	13174505	1
Caelo	Castor oil	13196308	1
Caelo	Castor oil	13357506	1
Noweda	Castor oil	13196313	1
Caelo	Castor oil	13I27-B01-287858	1
Fagron	Castor oil	13I27-B01-287858	1
Fagron	Castor oil	13I27-B01-287857	1
Fagron	Castor oil	13G29-B01-285422	1
Fagron	Castor oil	13G29B01	1
Caelo	Castor oil	14020101	1
Caelo	Castor oil	14020104	2
Fagron	Castor oil	13L27B01287857	1
Caelo	Castor oil	14020105	3
Caelo	Castor oil	14020106	2
Caelo	Castor oil	14020108	9
Fagron	Castor oil	14020108	1
Caelo	Castor oil	14020109	5
AHD/Caealo 15.08.14	Castor oil	14020109	1
Phönix	Castor oil	1403024-01	1
Euro OTC	Castor oil	1403024-02	6
Euro OTC	Castor oil	140302402	1
Euro OTC	Castor oil	140705301	1
Ph.Eur.8.0	Castor oil	140705301	1
Eur	Castor oil	1407053-01	1
Fagron	Castor oil	1407053-02	1
Euro OTC	Castor oil	1407053-02	7
Castor Pruducts Company...	Castor oil	1407053-02	1
Caelo	Castor oil	1412006-01	1
Euro OTC	Castor oil	141200601	1
Bombastus	Castor oil	1412006-01	1
Caelo	Castor oil	1412006-02	2
Euro/Noweda	Castor oil	1412006-02	1
Euro OTC	Castor oil	141200602	2
Caelo	Castor oil	14181102	1

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Supplier	Substance	Batch	Spectra
Caelo	Castor oil	14181103	2
Caelo	Castor oil	14199507	2
Caelo	Castor oil	14199602	1
Caelo	Castor oil	14199604	4
AHD	Castor oil	14199604	2
Caelo	Castor oil	14199605	4
Caelo	Castor oil	14199609	6
Caelo	Castor oil	14199609	1
Caelo	Castor oil	1420106	1
Caelo	Castor oil	14330601	1
Caelo	Castor oil	14304803	2
Fagron	Castor oil	14330601	1
Caelo	Castor oil	14304806	1
Caelo	Castor oil	14330604	6
Caelo	Castor oil	14304807	1
Caelo	Castor oil	14330605	3
Caelo	Castor oil	14330606	10
Fagron	Castor oil	14C17-B01	3
Caelo	Castor oil	15/355/Ri	1
Fagron	Castor oil	14C17-B01-293834	1
Fagron	Castor oil	14c17-b01-293832	1
Euro OTC	Castor oil	1504006-01	1
Sanacorp	Castor oil	1504006-01	1
EuRho / 11	Castor oil	1504006-02	2
Euro OTC	Castor oil	1504006-02	3
Fagron	Castor oil	1504006-01	1
Euro OTC	Castor oil	150400602	1
Caelo	Castor oil	150400602	1
Unisan	Castor oil	1504006-02	1
Anzag/Henry Lamotte	Castor oil	1504006-02	1
Phönix Gotha	Castor oil	1509003-01	1
Euro OTC	Castor oil	150900301	1
Euro OTC	Castor oil	1512024-01	5
Euro OTC	Castor oil	151204-02	1
Caelo	Castor oil	15144302	2
Caelo	Castor oil	15144303	2
Caesar&Loretz/Caesar&Lo...	Castor oil	15144304	1
Caelo	Castor oil	15144305	1
Caelo	Castor oil	15144307	2
Caelo	Castor oil	15145101	4
Rondell Apotheke	Castor oil	15145101	1
Caelo	Castor oil	15145104	1
Caelo	Castor oil	15145105	1
Fagron	Castor oil	1528-B07-3048	1
Caelo	Castor oil	15253403	1
Caelo	Castor oil	15392003	2
Caelo	Castor oil	15392002	1
Caelo	Castor oil	15392007	2
Fagron	Castor oil	15A28-B07-304816	1
Fagron	Castor oil	15A28B07	1
Euro OTC	Castor oil	154006-02	1
Fagron	Castor oil	15D02-B02-311714	2
Fagron	Castor oil	15A28-B07-304818	1
Fagron	Castor oil	15J15-B08	1
Sanacorp	Castor oil	15D02-Bo2-311714	1
Fagron	Castor oil	15J15-B08-318730	1
Caelo	Castor oil	15J15-B08-318730	1
Caelo	Castor oil	16016203	1
Caelo	Castor oil	16/081/R	1
Anzag	Castor oil	16016207	1

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Supplier	Substance	Batch	Spectra
Caelo	Castor oil	1604019-01	1
Caelo	Castor oil	16102801	2
Caelo	Castor oil	16102802	3
Fagron	Castor oil	16C29-B01-320886	1
Caelo	Castor oil	18021505	1
Caelo	Castor oil	16236205	1
Caelo	Castor oil	1913A-02009	1
Caelo	Castor oil	26041403	1
Caelo	Castor oil	24101402	1
Bombastus	Castor oil	268699	1
Gehe 05.03.2014	Castor oil	278660	1
Caelo	Castor oil	28051512	1
Bom	Castor oil	280791	1
Sanacorp	Castor oil	281943	1
Bombastu-Werke AG/Gehe	Castor oil	281944	1
Gehe	Castor oil	283620	3
Bombastus	Castor oil	283620	5
Bombastus	Castor oil	284505	6
Bombastus	Castor oil	285757	2
GEHE 17.07.2014	Castor oil	285757	1
Caelo	Castor oil	284505	2
Bombastus	Castor oil	285801	9
Bombastus	Castor oil	287167	9
Caelo	Castor oil	287167	2
Bombastus	Castor oil	288126	7
Bombasus/ Anzag	Castor oil	288126	1
Gehe	Castor oil	288126	1
Caelo	Castor oil	288126	1
Bombastus	Castor oil	288638	2
Gehe Kassel	Castor oil	288638	2
Bombastus	Castor oil	288639	11
lamotte Phoenix	Castor oil	288721	1
Gehe Kassel 06.06.2015	Castor oil	290212	1
Bombastus	Castor oil	290213	11
Hedinger/Sanacorp	Castor oil	290213	1
Caelo	Castor oil	292409	1
Bombastus	Castor oil	294667	3
Caelo	Castor oil	294667	1
Caelo	Castor oil	294668	1
Caelo	Castor oil	295412	2
Fagron	Castor oil	294668	1
Caelo	Castor oil	296751	3
Bombastus	Castor oil	297430	7
Caelo	Castor oil	298698	1
Caelo	Castor oil	30031504	1
Caelo	Castor oil	300629	1
Bombastus	Castor oil	301590	2
Bombastus	Castor oil	301591	5
Caelo	Castor oil	301591	1
Caelo	Castor oil	4614M-02009	1
Fagron	Castor oil	301591	1
Bombastus	Castor oil	303857	1
Bombastus	Castor oil	303858	1
Henry Lamotte Oils GmbH	Castor oil	5450801	1
Henry Lamotte/ Noweda	Castor oil	5450801	2
Phönix/Lamotte	Castor oil	5450801	13
Lamotte/L3	Castor oil	5450801	1
Henry Lamotte Oils, Gehe	Castor oil	5450801	1
Henry Lamotte/Gehe	Castor oil	5450801	2
Fagron	Castor oil	5450801	1

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Supplier	Substance	Batch	Spectra
Henry Lamotte Oils/GEHE	Castor oil	5899201	1
Noweda/Henry Lamotte	Castor oil	5899201	2
lamotte/Phönix	Castor oil	5899201	1
Bombastus	Castor oil	91696	1
Caelo	Castor oil	5899201	1
Euro OTC	Castor oil	60082103	1
Ichthyol	Castor oil		1
Fagron	Castor oil		1
Caelo	Castor oil	1206039-01	1
Caelo	Castor oil	1/AKD1	1
Caelo	Castor oil	11359507	1
Eurho / Sanacorp	Castor oil	121008-02	1
Euro OTC	Castor oil	126279	1
Fagron	Castor oil	12D04-N09	2
Bergchemie	Castor oil	13096304	1
Euro OTC	Castor oil	3313U-03553	1
Cealo	Castor oil	13096304	1
Fagron	Castor oil	13D29-N01	1
Euro OTC	Castor oil	1513A03553	2
Euro OTC	Castor oil	3513I-03553	1
Caelo	Castor oil	269565	1
Bombastus	Castor oil	268877	1
Bombastus	Castor oil	271753	2
Bombastus	Castor oil	273389	1
Noweda	Castor oil	273390	1
Phönix 07.12.12	Castor oil	273390	1
Caelo	Castor oil	272591	1
Phoenix 21.03.13	Castor oil	273881	2
Bombastus	Castor oil	273881	2
Caelo	Castor oil	11359508	1
Euro OTC	Castor oil	1202041-01	1
Geo-Chem/sanacorp	Castor oil	1206039-01	1
Euro OTC	Castor oil	1206039-02	1
Caelo	Castor oil	12071107	1
Geo-Chem/sanacorp	Castor oil	1212008-01	1
Sanacorp	Castor oil	12149306	1
Caelo	Castor oil	15012016	1
gehe, 18.01.2013	Castor oil	272591	1
Gehe	Castor oil	275937	1
Gehe	Castor oil	275938	2
Caelo	Castor oil	275938	3
Bombastus	Castor oil	278660	3
Noweda / Henry Lamotte	Castor oil	5280301	1
Lamotte	Castor oil	5188401	1
HenryLamotte/Phoenix	Castor oil	5280301	1
Otto Fischar Gmbh	Castor oil	5334001	1
Henry Lamotte	Castor oil	5334001	1
Lamotte	Castor oil	5334001	2
Henry Lamotte Oils	Castor oil	5334001	1
lamotte	Castor oil	5450801	1
lamotte/anzag	Castor oil	5334001	1
Ph.Eur.	Castor oil	6861795	1
Bombastus	Castor oil	60082103	1

- 57 450 spectra from 332 *Apo-Ident* customers from a total of 19 897 batches from a further 328 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 *Castor 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 *Castor 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	285	0	34 059
Type B	0	635	0	62 959
Type C	0	989	2	57 338

The substance/substance group *Castor 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 % (> 99.9689 %)	100.0000 % (> 97.8947 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 99.0551 %)
Type C	100.0000 % (> 99.5964 %)	99.7982 % (> 99.4955 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30741	31343	1.99	46.19
31343	31343	0.00	48.63
31739	31739	0.00	46.33
31751	31739	1.76	46.69
31824	31739	0.81	45.75
31845	31845	0.00	44.68
32943	31739	4.17	47.63

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Cedar leaf oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31106-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Cedar leaf oil; Oleum cedri e fol. aether.

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 leaf oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cedar leaf oil	13337901	31106	40	1404622
Caelo	Cedar leaf oil	13337901	31200	40	20131011
Caelo	Cedar leaf oil	13337902	31421	40	20131011

Validation samples

A total of 156 379 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 *Cedar leaf oil*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 32 spectra of 2 reference samples from the substance/substance group *Cedar leaf oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cedar leaf oil	13337902	31421 [†]	20
Caelo	Cedar leaf oil	15305206	not required	12

- 63 562 spectra from a total of 1475 batches from further 439 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 *Cedar leaf oil*.
- 58 441 spectra from 332 *Apo-Ident* customers from a total of 20 092 batches from a further 329 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](#).

[†]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*.

Validation results

The validation runs checked whether the substance/substance group *Cedar leaf 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 leaf 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	34 224
Type B	0	32	0	63 562
Type C	0	0	0	58 441

The substance/substance group *Cedar leaf 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 81.2500 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31106	31106	0.00	84.29
31200	31106	1.38	85.62
31421	31106	2.18	86.93

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Cedar wood oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30938-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cedar wood oil; Oleum cedri ligni aether.

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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
Caelo	Cedar wood oil	12180708	30938	50	1404506
Caelo	Cedar wood oil	12180710	31267	40	20120628
Caelo	Cedar wood oil	14230204	32455	40	1610271

Validation samples

A total of 156 379 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 *Cedar wood oil*. These samples are listed above in the [calibration samples](#) section.
- 34 214 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 1 reference samples from the substance/substance group *Cedar wood oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cedar wood oil	14230211	32748	40

- 63 554 spectra from a total of 1476 batches from further 439 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 *Cedar wood oil*.

Supplier	Substance	Batch	Spectra
Caelo	Cedar wood oil	12180709	1
Caelo	Cedar wood oil	12180710	1
Caelo	Cedar wood oil	12180703	1

- 58 438 spectra from 332 *Apo-Ident* customers from a total of 20 089 batches from a further 328 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	130	0	34 214
Type B	0	40	0	63 554
Type C	0	2	1	58 438

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 % (> 99.9691 %)	100.0000 % (> 95.3846 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.5993 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30938	30938	0.00	24.69
31267	30938	1.99	25.03
32455	32455	0.00	31.39

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Cinnamon bark oil, artificial**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30605-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Cinnamon bark oil, artificial; Oleum Cinnamomi artificiale

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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, artificial*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cinnamon bark oi...	11275903	30605	40	1402333
Caelo	Cinnamon bark oi...	14377301	31617	40	20150107

Validation samples

A total of 156 379 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 *Cinnamon bark oil, artificial*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 20 spectra of 1 reference samples from the substance/substance group *Cinnamon bark oil, artificial*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cinnamon bark oil, artificial	14377301	31617 [†]	20

- 63 574 spectra from a total of 1476 batches from further 439 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 6 *Apo-Ident* customers from 6 batches from the substance/substance group *Cinnamon bark oil, artificial*.

Supplier	Substance	Batch	Spectra
Caelo	Cinnamon bark oil, artificial	14377304	1
Caelo	Cinnamon bark oil, artificial	2031501	1
Caelo	Cinnamon bark oil, artificial	14377307	1

continued on the next page

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

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Supplier	Substance	Batch	Spectra
Caelo	Cinnamon bark oil, artificial	10112014	1
Caelo	Cinnamon bark oil, artificial	11275903	1
Caelo	Cinnamon bark oil, artificial	12019604	1

- 58 435 spectra from 332 *Apo-Ident* customers from a total of 20 086 batches from a further 328 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, artificial* 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, artificial* 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	34 264
Type B	0	20	0	63 574
Type C	0	5	1	58 435

The substance/substance group *Cinnamon bark oil, artificial* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9712 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.5978 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30605	30605	0.00	18.55
31617	30605	3.75	17.86

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Cinnamon bark oil, Ceylon
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30251-2017-07-04
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:

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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
Caelo	Cinnamon bark oi...	11352506	30604	40	20111219
Caelo	Cinnamon bark oi...	14092802	31560	40	AR-15-FG-001171-01
Caelo	Cinnamon bark oi...	163243	33091	40	20161129*

Validation samples

A total of 156 379 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 *Cinnamon bark oil, Ceylon*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Cinnamon bark oil, Ceylon*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cinnamon bark oil, Ceylon	10185201	30251	40
Caelo	Cinnamon bark oil, Ceylon	14092802	31560 [†]	20

- 63 534 spectra from a total of 1475 batches from further 439 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.

- 29 spectra from 19 *Apo-Ident* customers from 18 batches from the substance/substance group *Cinnamon bark oil, Ceylon*.

*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.

[†]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*.

Supplier	Substance	Batch	Spectra
Apotheke in Steinkuhl	Cinnamon bark oil, Ceylon	110504/3	1
Caelo	Cinnamon bark oil, Ceylon	12181408	1
Ölbaum / Anzag	Cinnamon bark oil, Ceylon	10220032803	1
Caelo	Cinnamon bark oil, Ceylon	11352506	1
Taoasis	Cinnamon bark oil, Ceylon	130111-110762	2
Caelo	Cinnamon bark oil, Ceylon	13044802	4
/Noweda	Cinnamon bark oil, Ceylon	13044802	4
Caelo	Cinnamon bark oil, Ceylon	13044810	3
Caelo	Cinnamon bark oil, Ceylon	11352501	1
Taoasis GmbH	Cinnamon bark oil, Ceylon	130111-110345	1
Caelo	Cinnamon bark oil, Ceylon	14071203	1
Caelo	Cinnamon bark oil, Ceylon	13044808	1
Caelo	Cinnamon bark oil, Ceylon	13044809	1
Dr.Schlegels Resana/NOW	Cinnamon bark oil, Ceylon	1205-3566	1
Dr.Schlegels Resana/NOW	Cinnamon bark oil, Ceylon	1407-4584	1
Caelo	Cinnamon bark oil, Ceylon	14092802	1
Caelo	Cinnamon bark oil, Ceylon	14092805	2
Caelo	Cinnamon bark oil, Ceylon	12181403	1
Caelo	Cinnamon bark oil, Ceylon	14092806	1

- 58 412 spectra from 332 *Apo-Ident* customers from a total of 20 074 batches from a further 328 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	120	0	34 224
Type B	0	60	0	63 534
Type C	0	25	4	58 412

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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.5966 %)	86.2069 % (> 75.8621 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30604	31560	5.78	33.98
31560	31560	0.00	34.16
33091	33091	0.00	28.72

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Citronella oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30208-2017-07-04
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:

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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
Caelo	Citronella oil	12359903	31251	40	1405526
Caelo	Citronella oil	13287808	31408	40	20130827
Caelo	Citronella oil	14229803	31631	40	20140825

Validation samples

A total of 156 379 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 *Citronella oil*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 141 spectra of 4 reference samples from the substance/substance group *Citronella oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citronella oil	9323007	30208	41
Caelo	Citronella oil	91668379	30250	40
Caelo	Citronella oil	14229803	31631 [†]	20
Caelo	Citronella oil	162791	32692	40

- 63 453 spectra from a total of 1473 batches from further 439 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 22 *Apo-Ident* customers from 27 batches from the substance/substance group *Citronella oil*.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Citronella oil	12359903	2
Caelo	Citronella oil	12359907	1
Caelo	Citronella oil	13287802	1
Caelo	Citronella oil	13287808	1
Caelo	Citronella oil	15257304	1
Caelo	Citronella oil	14229805	1
Caelo	Citronella oil	286270	1
Phönix Gotha	Citronella oil	288826	1
Bombastus	Citronella oil	286270	1
Bergland	Citronella oil	C400822	1
Caelo	Citronella oil	15222303	1
Caelo	Citronella oil	15257305	1
Caelo	Citronella oil	15257308	1
Caelo	Citronella oil	10193312	1
Bombastus	Citronella oil	302908	1
Caelo	Citronella oil	11101301	1
Caelo	Citronella oil	11074201	1
Bombastus	Citronella oil	1213A-01974	1
Caelo	Citronella oil	11074203	1
Euro OTC	Citronella oil	12224603	1
Caelo	Citronella oil	12359902	1
Caelo	Citronella oil	12359909	1
Caelo	Citronella oil	13287804	1
Kaders	Citronella oil	131097	1
Bombastus	Citronella oil	276241	1
Caelo	Citronella oil	276241	1
Bombastus	Citronella oil	280657	1
Phönix Gotha	Citronella oil	260477	1
Bombastus	Citronella oil	269807	1

- 58 411 spectra from 332 *Apo-Ident* customers from a total of 20 066 batches from a further 328 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	120	0	34 224
Type B	0	115	26	63 453
Type C	0	29	1	58 411

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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9710 %)	81.5603 % (> 79.4326 %)
Type C	100.0000 % (> 99.5966 %)	96.6667 % (> 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.

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
31251	31251	0.00	41.51
31408	31251	7.14	41.88
31631	31251	2.39	42.48

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Citrus oils
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31017-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrus oils; Bitter orange peel oil; Citric oil; Grapefruit oil; Limonis aetheroleum; Oleum aurantii dulcis; Oleum aurantii pericarpium; Oleum citri; Oleum citri paradisi artificiale; Sweet orange peel oil

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Citrus oils*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Grapefruit oil	12367403	31017	40	1404621
Fagron	Citric oil	13E06-N10	31046	40	20130618
Caelo	Sweet orange pee...	12043412	31164	40	1405105

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sweet orange pee...	13378901	31206	40	1405107
Fagron	Citric oil	12G13-B06-287454	31261	40	1407356
Caelo	Sweet orange pee...	13024204	31273	40	20130124
Caelo	Sweet orange pee...	13378906	31295	40	1407188
Caelo	Sweet orange pee...	13401605	31297	38	20131220
Caelo	Sweet orange pee...	13024204	31411	40	20130124
Caelo	Grapefruit oil	13252306	31417	40	20130802
Caelo	Sweet orange pee...	13378906	31418	40	20131127
Caelo	Citric oil	13259522	31432	40	20130816
Euro OTC	Citric oil	1202024-01	31524	40	20120312
Caelo	Bitter orange pe...	13303803	31861	40	1606482
Caelo	Bitter orange pe...	15397901	32181	40	20151125
Caelo	Bitter orange pe...	170369	33062	30	20170224*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 628 spectra of 16 reference samples from the substance/substance group *Citrus oils*. These samples are listed above in the [calibration samples](#) section.
- 33 716 spectra from a total of 784 batches from further 221 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 240 spectra of 9 reference samples from the substance/substance group *Citrus oils*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sweet orange peel oil	9319501	30171	40
Caelo	Citric oil	90965219	30248	20
Caelo	Grapefruit oil	13252306	31417 [†]	20
Caelo	Sweet orange peel oil	13378906	31418 [†]	20
Caelo	Citric oil	13259522	31432 [†]	20
Euro OTC	Citric oil	1202024-01	31524 [†]	20
Caelo	Bitter orange peel oil	13303803	31861 [†]	20
Caelo	Bitter orange peel oil	15397901	32351	40
Caelo	Citric oil	162752	32687	40

*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.

- 63 354 spectra from a total of 1468 batches from further 436 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.

- 239 spectra from 95 *Apo-Ident* customers from 124 batches from the substance/substance group *Citrus oils*.

Supplier	Substance	Batch	Spectra
Taoasis	Citric oil	4LI14M-118369	1
Fagron	Citric oil	11C28-N060363/440	2
Taoasis	Citric oil	122527-122620	1
Caelo	Citric oil	12360012	5
Fagron	Citric oil	12G13-B06-287454	1
Caelo	Citric oil	13259508	7
Caelo	Citric oil	13259504	7
Caelo	Citric oil	13259523	4
Fagron	Citric oil	13B01N02	2
Fagron	Citric oil	13E06-N10	6
Fagron	Citric oil	13K14-B03-289819	1
Fagron	Citric oil	13K14-B03-294706	3
Taoasis	Citric oil	1401270-121612	1
Fagron	Citric oil	13K14-B03-787033	1
Taoasis	Citric oil	140116-115338	1
Caelo	Citric oil	14121807	3
Caelo	Citric oil	14121813	1
Caelo	Citric oil	14121815	4
Caelo	Citric oil	14H06-B02	1
Caelo	Citric oil	14365212	4
Fagron	Citric oil	14H06-B02-299949	2
Caelo	Citric oil	15121403	1
Caelo	Citric oil	15182703	7
Bombastus	Citric oil	280999	4
Bombastus	Citric oil	284045	1
Caelo	Citric oil	288778	1
Bombastus	Citric oil	289673	1
Bombastus	Citric oil	294337	1
Sanacorp	Citric oil	5/AKD1	1
Taoasis	Citric oil	5LI12M-109229	1
Sanacorp	Citric oil		1
Caelo	Citric oil	9322802	1
Caelo	Citric oil	9322807	1
Caelo	Citric oil	9322815	1
Noweda	Citric oil	10375003	2
Caelo	Citric oil	10375003	2
Caelo	Citric oil	11231807	2
Caelo	Citric oil	10375014	1
Caelo	Citric oil	1135408	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
Caelo	Citric oil	10375012	1
Fagron	Citric oil	11B04-N02	2
Fagron	Citric oil	11D28-N09	1
Fagron	Citric oil	11K28-N04	2
Fagron	Citric oil	11K28-N04	1
Caelo	Citric oil	12040502	4
Fagron	Citric oil	11I05-N13	1
DEFEKTUR	Citric oil	1202024-01	1
Caelo	Citric oil	12040504	8
Sanacorp	Citric oil	12040504	1
Anzag 15.11.12 ek:17,18	Citric oil	12040507	1
Caelo	Citric oil	12360002	5
Taoasis	Citric oil	122650-123634	1
Anzag 17.06.2013	Citric oil	12360001	1
Caelo	Citric oil	12040507	1
Caelo	Citric oil	123600002	1
Caelo	Citric oil	12360001	1
Caelo	Citric oil	123600001	1
Noweda	Citric oil	12360002	1
Cealo	Citric oil	12360002	1
Caelo	Citric oil	12360010	2
Caelo	Citric oil	12360010c	1
Caelo	Citric oil	12360011	10
Caelo	Citric oil	12360012x2	1
Fagron	Citric oil	12A23-N05	7
Caelo	Citric oil	12360013	1
Fagron	Citric oil	12G04-N21	2
Fagron	Citric oil	12A23-N05	1
Caelo	Citric oil	132259504	1
Caelo	Citric oil	1359512	1
Gehe 29.04.2013	Citric oil	13B01N/02	1
Fagron	Citric oil	13B01-N02	6
Fagron	Citric oil	13b01-n02	1
Caelo	Citric oil	15051314	1
Caelo	Citric oil	13E06-N100875/900	1
Caelo	Citric oil	2515I-01973	1
Caelo	Citric oil	20111307	1
Fagron	Citric oil	268961	1
Caelo	Citric oil	15182711	1
Bombastus	Citric oil	266679	1
Caelo	Citric oil	28051308	1
Bombastus	Citric oil	297734	1
Taoasis	Citric oil	2LI08M-73396	1
Caelo	Citric oil	3710A-01973	1
Caelo	Citric oil	31121206	1
Taoasis	Citric oil	3805201	1
Fagron	Citric oil	602796	1
Fagron	Citric oil	645920	4
Caelo	Grapefruit oil	13252303	1
Caelo	Grapefruit oil	13252306	1
Caelo	Grapefruit oil	14107304	1
Taoasis	Grapefruit oil	31564-120540	1
Apotheker-Bauer	Grapefruit oil		1
Taoasis	Grapefruit oil	333555-111392	1
Bombastus	Citric oil	285568	1
Fagron	Citric oil	13K14-B03	2
Caelo	Sweet orange peel oil	13024204	4
Caelo	Grapefruit oil	12367403	1
Fagron	Citric oil	12g13-b06-287454	1
Fagron	Citric oil	14H06-B02	1

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Supplier	Substance	Batch	Spectra
Bombastus	Citric oil	256839	1
Sanacorp	Citric oil	13259504	1
Bombastus	Citric oil	269281	1
Bombastus	Citric oil	284351	1
Caelo	Bitter orange peel oil	15397903	1
Nachprüfung	Sweet orange peel oil	12043403	5
Caelo	Sweet orange peel oil	12043406	1
Caelo	Sweet orange peel oil	13389406	3
Caelo	Sweet orange peel oil	12043409	1
Taoasis	Sweet orange peel oil	140129-115917	1
Caelo	Sweet orange peel oil	14348803	3
Caelo	Sweet orange peel oil	14133505	1
Caelo	Sweet orange peel oil	15182904	1
Caelo	Sweet orange peel oil	15051701	1
Caelo	Sweet orange peel oil	15045101	1
Caelo	Sweet orange peel oil	14348809	1
Caelo	Sweet orange peel oil	15316601	1
Primavera	Sweet orange peel oil	530914	1
Caelo	Sweet orange peel oil	15285	1
Caelo	Sweet orange peel oil	7051301	1
Fiebig 09.11.12 ek:6,92	Sweet orange peel oil	11031802	1
Caelo	Sweet orange peel oil	8121204	1
Anzag	Sweet orange peel oil	11310411	1
Caelo	Sweet orange peel oil	10375113	1
Großhandel	Sweet orange peel oil	12043403	2
Caelo	Sweet orange peel oil	12043410	3
Caelo	Sweet orange peel oil	12322603	1
Caelo	Sweet orange peel oil	12322607	1
Caelo	Sweet orange peel oil	1302404	1
Caelo	Sweet orange peel oil	13024202	1
Caelo	Sweet orange peel oil	15051313	1
Caelo	Sweet orange peel oil	13389407	1
Caelo	Sweet orange peel oil	13389401	1
Phönix 16.05.2013	Sweet orange peel oil	271897	1
Bombastus	Sweet orange peel oil	271897	1

- 58 202 spectra from 332 *Apo-Ident* customers from a total of 19 968 batches from a further 325 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

The validation runs checked whether the substance/substance group *Citrus oils* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrus oils* 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	628	0	33 716
Type B	0	237	3	63 354
Type C	0	221	18	58 202

The substance/substance group *Citrus oils* 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 % (> 99.9689 %)	100.0000 % (> 99.0446 %)
Type B	100.0000 % (> 99.9710 %)	98.7500 % (> 97.5000 %)
Type C	100.0000 % (> 99.5963 %)	92.4686 % (> 91.2134 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31017	31017	0.00	43.10
31046	31261	10.13	36.52
31164	31164	0.00	43.24
31206	31206	0.00	46.25
31261	31261	0.00	31.46
31273	31206	2.65	49.74
31295	31295	0.00	47.08
31297	31295	2.50	50.48
31411	31295	1.71	48.93
31417	31164	2.36	46.51
31418	31295	1.85	48.02
31432	31261	2.16	31.12
31524	31261	5.21	31.18
31861	31861	0.00	30.04
32181	31861	8.64	40.03
33062	33062	0.00	39.20

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Clotrimazole 10% Cordes® RK**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30213-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Clotrimazole 10% Cordes® RK

Special notes

When selecting the *Clotrimazole 10% Cordes® RK* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Clotrimazole 10% Cordes® RK*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Ichthyol	Clotrimazole 10%...	11D044	30729	40	20111213
Ichthyol	Clotrimazole 10%...	12D016	31101	40	1507525
Ichthyol	Clotrimazole 10%...	14D009	31806	40	20140606

Validation samples

A total of 156 379 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 *Clotrimazole 10% Cordes® RK*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 110 spectra of 3 reference samples from the substance/substance group *Clotrimazole 10% Cordes® RK*.

Supplier	Substance	Batch	Sample ID	Spectra
Ichthylol	Clotrimazole 10% Cordes® RK	9D036	30213	50
Ichthylol	Clotrimazole 10% Cordes® RK	14D009	31806 [†]	20
Ichthylol	Clotrimazole 10% Cordes® RK	14D009	32950	40

- 63 484 spectra from a total of 1475 batches from further 439 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.

- 36 spectra from 16 *Apo-Ident* customers from 8 batches from the substance/substance group *Clotrimazole 10% Cordes® RK*.

Supplier	Substance	Batch	Spectra
Ichthylol/Alliance Healt...	Clotrimazole 10% Cordes® RK	120016	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
Ichthyol-Gesellschaft/N...	Clotrimazole 10% Cordes® RK	110044	1
Ichthyol/Jenne	Clotrimazole 10% Cordes® RK	12D016	11
Ichthyol/Noweda	Clotrimazole 10% Cordes® RK	12D016	3
Ichthyol	Clotrimazole 10% Cordes® RK	12D016	2
AHD/ichthyol	Clotrimazole 10% Cordes® RK	14D0089	1
Noweda	Clotrimazole 10% Cordes® RK	14D009	1
Ichthyol-Gesellschaft/ N...	Clotrimazole 10% Cordes® RK	14D009	2
ICHTHYOL-GESELLSCHAFT C...	Clotrimazole 10% Cordes® RK	14D009	1
Cordes	Clotrimazole 10% Cordes® RK	11D044	1
Ichthyol Gesellschaft C...	Clotrimazole 10% Cordes® RK	11D044	1
Ichthyol/Noweda	Clotrimazole 10% Cordes® RK	14D009	1
Ichthyol	Clotrimazole 10% Cordes® RK	11D044	1
Ichthyol4D/ Noweda	Clotrimazole 10% Cordes® RK	14D009	1
Ichthyol/Jenne	Clotrimazole 10% Cordes® RK	11D044	1
Ichthyol Gesellschaft C...	Clotrimazole 10% Cordes® RK	11D044	1
Ichthyol-Gesellschaft/G...	Clotrimazole 10% Cordes® RK	12D016	2
Ichthyol	Clotrimazole 10% Cordes® RK	11D044	1
Ichthyol/ Noweda	Clotrimazole 10% Cordes® RK	12D016	1
Ichthyol-Gesellschaft / K	Clotrimazole 10% Cordes® RK	12D016	1
Ichthyol Noweda	Clotrimazole 10% Cordes® RK	12D016	1

- 58 405 spectra from 332 *Apo-Ident* customers from a total of 20 084 batches from a further 328 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 *Clotrimazole 10% Cordes® RK* 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 *Clotrimazole 10% Cordes® RK* 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	34 224
Type B	0	110	0	63 484
Type C	0	36	0	58 405

The substance/substance group *Clotrimazole 10% Cordes® RK* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 94.5455 %)
Type C	100.0000 % (> 99.5965 %)	100.0000 % (> 83.3333 %)

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

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

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30729	31101	4.93	82.78
31101	31101	0.00	81.06
31806	31101	18.57	93.74

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Clove oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30858-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Clove oil; Caryophylli floris aetheroleum; Oleum caryophylli

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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
Caelo	Clove oil	12165905	30858	40	20120627
Caelo	Clove oil	13334902	31299	40	20131009
Caelo	Clove oil	13334902	31409	40	20131009
Euro OTC	Clove oil	1210057-01	31526	40	AR-14-FG-013260-01
Euro OTC	Clove oil	1505022	31707	40	0000010252

Validation samples

A total of 156 379 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 *Clove oil*. These samples are listed above in the [calibration samples](#) section.
- 34 144 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Clove oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Clove oil	1210057-01	31526 [†]	20
Euro OTC	Clove oil	1505022	31707 [†]	20

- 63 554 spectra from a total of 1475 batches from further 439 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.

- 297 spectra from 103 *Apo-Ident* customers from 103 batches from the substance/substance group *Clove oil*.

Supplier	Substance	Batch	Spectra
Caelo	Clove oil	14243105	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
Caelo	Clove oil	14243104	11
Caelo	Clove oil	11231706	8
Caelo	Clove oil	15119303	2
Caelo	Clove oil	12380601	8
Fischar/Gehe	Clove oil	13334905	1
Caelo	Clove oil	13334905	6
Caelo	Clove oil	13334902	11
Caelo	Clove oil	14133602	4
Caelo	Clove oil	10272002	3
Caelo	Clove oil	15316103	6
Caelo	Clove oil	11231702	8
Caelo	Clove oil	11231704	4
Caelo	Clove oil	12165905	1
Caelo	Clove oil	12165902	6
phönix 30.07.2013	Clove oil	12165905	1
Caelo	Clove oil	13182301	20
Caelo	Clove oil	13106501	13
Caelo	Clove oil	12165905	13
Caelo	Clove oil	13106502	4
Caelo	Clove oil	2081402	1
Fagron	Clove oil	204211969	1
Fagron	Clove oil	208211969	1
Caelo	Clove oil	4061404	1
Caelo	Clove oil	2091306	1
Caelo	Clove oil	6071501	1
Caelo	Clove oil	10272012	3
Caelo	Clove oil	10272014	2
Anzag 03.07.2012	Clove oil	1108015-01	1
Euro OTC	Clove oil	1108015-01	2
Noweda	Clove oil	11231702	2
Phoenix, 31.08.2012	Clove oil	11231702	1
Caelo	Clove oil	11231703	4
Anzag am 03.07.2012	Clove oil	11231703	1
11231703	Clove oil	11231703	1
Fagron	Clove oil	11K17-N07	1
Caelo	Clove oil	11231709	2
Phönix 21.12.12	Clove oil	11K17-N07	1
Fagron	Clove oil	11L21-N07	2
phönix 22.01.2013	Clove oil	11L21-N07	1
Euro OTC	Clove oil	1206012-01	1
Euro OTC	Clove oil	1206013-01	8
Phönix, 21.12.2012	Clove oil	11L21N07	1
Caelo	Clove oil	12011502	1
Euro OTC	Clove oil	1210057-01	1
Euro OTC	Clove oil	121005701	1
EuRho	Clove oil	1210057-01	2
Euro/Gehe	Clove oil	1210057-01	1
Caelo	Clove oil	121655905	1
Caesar/Noweda	Clove oil	12165902	1
Noweda	Clove oil	12165905	3
Sanacorp	Clove oil	12165905	1
Phönix	Clove oil	12165905	1
Caelo	Clove oil	12272004-1-0	1
Fagron	Clove oil	12C27-N04	1
Caelo	Clove oil	123806012x	1
Taoasis	Clove oil	130301-110695	2
gehe, 10.01.2013	Clove oil	130110	1
Fagron	Clove oil	12F01-N01	2
phönix 14.08.2013	Clove oil	12C27-N04	1
Calo	Clove oil	13106501	1

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Supplier	Substance	Batch	Spectra
Gehe	Clove oil	13106501	1
phönix 30.07.2013	Clove oil	13182301	1
Noweda	Clove oil	13334902	1
Caesar/Noweda	Clove oil	13334905	1
Phonix	Clove oil	13334905	1
Fagron	Clove oil	13L03-B01294950	1
Caelo	Clove oil	14133603	4
Caelo	Clove oil	14133608	3
Caelo	Clove oil	14243101	3
Caelo	Clove oil	14243103	6
Caelo	Clove oil	14243102	1
Caelo	Clove oil	15051508	1
Caelo	Clove oil	15119304	9
Caelo	Clove oil	15101401	1
Caelo	Clove oil	15101402	1
Fagron	Clove oil	1512211969	1
Caelo	Clove oil	15316101	1
Caelo	Clove oil	15316102	13
Phoenix	Clove oil	15316102	1
Caelo	Clove oil	16121305	1
Caesar & Loretz	Clove oil	15402102	1
Caelo	Clove oil	18071302	1
Caelo	Clove oil	18121411	1
Caelo	Clove oil	265130	1
Caelo	Clove oil	23041404	1
Caelo	Clove oil	23051405	1
Caelo	Clove oil	17051402	1
Caelo	Clove oil	23081402	1
Bombastus	Clove oil	265673	1
Caelo	Clove oil	20021308	1
Caelo	Clove oil	267700	1
Bombastus	Clove oil	267699	1
Bombastus	Clove oil	272735	1
Caelo	Clove oil	272735	2
Bombastus	Clove oil	273027	1
Bombastus	Clove oil	274495	1
Großhandel	Clove oil	273462	2
Bombastus	Clove oil	274829	1
Bombastus	Clove oil	279262	2
Caelo	Clove oil	28051313	1
Bombastus	Clove oil	285572	1
Caelo	Clove oil	28051510	1
Bombastus	Clove oil	288127	1
Caelo	Clove oil	294000	2
Bombastus	Clove oil	288875	1
Bombastus	Clove oil	297263	1
Bombastus	Clove oil	296979	1
Bombastus	Clove oil	295672	1
Caelo	Clove oil	30111304	1
Caelo	Clove oil	3512M-01969	1
Bombastus	Clove oil	300901	1
Taoasis/ Sanacorp	Clove oil	B130612-112414	1
Fagron	Clove oil	3113Q01969	1
Wolf	Clove oil	6811	1
Euro OTC	Clove oil	5210A-01969	1
Caelo	Clove oil	3613Q01969	1
Taoasis	Clove oil	97204	1
Caelo	Clove oil	0-130513-1	1
Caelo	Clove oil	11231705	1
Fagron	Clove oil	13L03-B01	1

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Supplier	Substance	Batch	Spectra
Fagron	Clove oil	13L03-B01-292270	1
Caelo	Clove oil	12165904	1
Caelo	Clove oil	11K17-No7	1
Fagron	Clove oil	11L21-N07	1
Fagron	Clove oil	12C27N04	1
Caelo	Clove oil	13182301-3373319042	1
Bombastus	Clove oil	60010610	1

- 58 144 spectra from 332 *Apo-Ident* customers from a total of 19 989 batches from a further 328 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	34 144
Type B	0	40	0	63 554
Type C	0	284	13	58 144

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 % (> 99.9690 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.5963 %)	95.6229 % (> 94.6128 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30858	31707	3.42	40.16
31299	31707	4.50	35.56
31409	31707	5.46	35.31
31526	31526	0.00	27.09
31707	31707	0.00	37.60

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Coal tar spirit SR
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31126-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Coal tar spirit SR; Lithanthracis picis spiritus SR; Spiritus picis lithanthracis SR

Special notes

When selecting the *Coal tar spirit SR* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Coal tar spirit SR*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Coal tar spirit SR	13D05-M14	31126	40	1403343
apomix	Coal tar spirit SR	04C151014	31626	40	20141022

Validation samples

A total of 156 379 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 *Coal tar spirit SR*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Coal tar spirit SR*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Coal tar spirit SR	2911015-01	30220	40
apomix	Coal tar spirit SR	4C151014	31626 [†]	20

- 63 534 spectra from a total of 1475 batches from further 439 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.

- 36 spectra from 26 *Apo-Ident* customers from 31 batches from the substance/substance group *Coal tar spirit SR*.

Supplier	Substance	Batch	Spectra
Gehe	Coal tar spirit SR	2B040413	1
Fagron	Coal tar spirit SR	11E18-M02	1
Fagron	Coal tar spirit SR	2A270215	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
Fagron	Coal tar spirit SR	2A070316	1
Gehe	Coal tar spirit SR	3B130614	1
apomix PKH GmbH Halle	Coal tar spirit SR	4A170615	1
Fagron	Coal tar spirit SR	3A130614	1
Apomix	Coal tar spirit SR	2C280414	1
pkh halle,phönix	Coal tar spirit SR	4A170615	1
gehe	Coal tar spirit SR	4B220813	1
Bombastus	Coal tar spirit SR	4C151014	1
Apomix / Alliance Healt...	Coal tar spirit SR	5B170715	1
PKH Halle / Anzag	Coal tar spirit SR	4C151014	1
PKH GmbH	Coal tar spirit SR	5B181113	1
Apomix	Coal tar spirit SR	5B170715	1
Apomix	Coal tar spirit SR	5B271112	1
Fagron	Coal tar spirit SR	14A30-M01	2
Caelo	Coal tar spirit SR	6A031213	1
Fagron	Coal tar spirit SR	13G16-M01	1
Caelo	Coal tar spirit SR	6B031213	1
Fagron	Coal tar spirit SR	14I04-M02	1
Fagron	Coal tar spirit SR	1404-M02	1
Apomix / Sanacorp	Coal tar spirit SR	2C040413	1
Gehe	Coal tar spirit SR	2B290212	1
apomix	Coal tar spirit SR	3C230508	1
apomix	Coal tar spirit SR	3b170412	1
Apomix/ Noweda	Coal tar spirit SR	6A211212	1
Apomix	Coal tar spirit SR	5A101210	1
ApoMix	Coal tar spirit SR	4B221009	1
Caelo	Coal tar spirit SR	5C271112	1
Gehe	Coal tar spirit SR	13D05-M14	1
Fagron	Coal tar spirit SR	13D05-M14	1
Gehe	Coal tar spirit SR	6B211212	1
Caelo	Coal tar spirit SR	15C11-M09	1
apomix	Coal tar spirit SR	7633599	1

- 58 405 spectra from 332 *Apo-Ident* customers from a total of 20 061 batches from a further 328 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 *Coal tar spirit 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 *Coal tar spirit 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	80	0	34 264
Type B	0	21	39	63 534
Type C	0	30	6	58 405

The substance/substance group *Coal tar spirit 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	35.0000 % (> 30.0000 %)
Type C	100.0000 % (> 99.5965 %)	83.3333 % (> 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.

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
31126	31126	0.00	97.55
31626	31126	5.65	98.35

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Collodion 4%
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30210-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Collodion 4%

Special notes

When selecting the *Collodion 4%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Collodion 4%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Collodion 4%	13325403	31186	40	1402569
Caelo	Collodion 4%	13325411	31434	40	20131016
Caelo	Collodion 4%	16284201	32962	40	20161107

Validation samples

A total of 156 379 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 *Collodion 4%*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 100 spectra of 3 reference samples from the substance/substance group *Collodion 4%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Collodion 4%	9247401	30210	40
Caelo	Collodion 4%	11336004	30533	40
Caelo	Collodion 4%	13325411	31434 [†]	20

- 63 494 spectra from a total of 1474 batches from further 439 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.

- 46 spectra from 21 *Apo-Ident* customers from 21 batches from the substance/substance group *Collodion 4%*.

Supplier	Substance	Batch	Spectra
Caelo	Collodion 4%	11336004	1
Caelo	Collodion 4%	13325403	2

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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
Caelo	Collodion 4%	7031404	1
Caelo	Collodion 4%	13325402	3
Caelo	Collodion 4%	13325405	3
Caelo	Collodion 4%	13325411	2
Caelo	Collodion 4%	14079101	3
Caesar&Loretz GmbH /Anzag	Collodion 4%	14079105	1
Caelo	Collodion 4%	14079105	2
Caelo	Collodion 4%	15199203	5
Euro OTC	Collodion 4%	14079105	1
Euro OTC	Collodion 4%	15199203	1
Caelo	Collodion 4%	15199206	1
Caesar & Loretz/Sanacorp	Collodion 4%	15199206	1
Caelo	Collodion 4%	16284201	1
Caelo	Collodion 4%	15429002	1
Caelo	Collodion 4%	27041502	1
Caelo	Collodion 4%	11336001	2
Caesar&loretz,Phoenix	Collodion 4%	12035916	1
Caelo	Collodion 4%	12035903	1
Caelo	Collodion 4%	12035913	1
Defektur	Collodion 4%	12035916	1
Caelo	Collodion 4%	12035916	5
Caelo	Collodion 4%	12220003	1
Caelo	Collodion 4%	20021305	1
Caelo	Collodion 4%	90266259	1
Caelo	Collodion 4%	13325401	1
Gehe	Collodion 4%	11336004	1

- 58 395 spectra from 332 *Apo-Ident* customers from a total of 20 071 batches from a further 328 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 *Collodion 4%* 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 *Collodion 4%* 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	34 224
Type B	0	87	13	63 494
Type C	0	43	3	58 395

The substance/substance group *Collodion 4%* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9710 %)	87.0000 % (> 84.0000 %)
Type C	100.0000 % (> 99.5965 %)	93.4783 % (> 86.9565 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31186	31186	0.00	169.28
31434	31186	10.79	172.90
32962	31186	25.22	173.32

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Contramarum aroma
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31007-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Contramarum aroma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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	20131230
Caelo	Contramarum aroma	13411007	31398	40	20131230

Validation samples

A total of 156 379 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 *Contramarum aroma*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 79 spectra of 2 reference samples from the substance/substance group *Contramarum aroma*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Contramarum aroma	11073903	30342	39
Caelo	Contramarum aroma	162671	32695	40

- 63 515 spectra from a total of 1475 batches from further 439 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 23 *Apo-Ident* customers from 28 batches from the substance/substance group *Contramarum aroma*.

Supplier	Substance	Batch	Spectra
Phoenix Goettin	Contramarum aroma	70401432001	1
Caelo	Contramarum aroma	2041515	1
Caelo	Contramarum aroma	1315Q-03148	1
Caelo	Contramarum aroma	13411007	4
Caelo	Contramarum aroma	13411002	1
Caelo	Contramarum aroma	14320006	3

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Supplier	Substance	Batch	Spectra
Caelo	Contramarum aroma	14320009	1
Caelo	Contramarum aroma	14320005	1
Caelo	Contramarum aroma	14320009	1
Caelo	Contramarum aroma	14320015	2
Caelo	Contramarum aroma	15113003	1
Caelo	Contramarum aroma	16083801	2
Caelo	Contramarum aroma	15113011	1
Caelo	Contramarum aroma	7091302	1
Caelo	Contramarum aroma	16083806	1
Caelo	Contramarum aroma	5315A-03148	1
Caelo	Contramarum aroma	21051508	1
Caelo	Contramarum aroma	11378804	1
Caelo	Contramarum aroma	7071207	1
Caelo	Contramarum aroma	16083802	1
Fiebig	Contramarum aroma	11378810	1
Gehe	Contramarum aroma	12201404	1
Gehe 08.05.2013	Contramarum aroma	12201407	1
Gehe 09.04.2013	Contramarum aroma	12201410	1
Caelo	Contramarum aroma	12201407	1
Caelo	Contramarum aroma	13141602	1
Cael	Contramarum aroma	13141603	1
Caelo	Contramarum aroma	13141606	3
Caelo	Contramarum aroma	13141608	2

- 58 402 spectra from 332 *Apo-Ident* customers from a total of 20 064 batches from a further 328 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	120	0	34 224
Type B	0	79	0	63 515
Type C	0	36	3	58 402

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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.4051 %)
Type C	100.0000 % (> 99.5965 %)	92.3077 % (> 84.6154 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31007	31007	0.00	53.27
31289	31007	7.04	50.32
31398	31007	5.79	51.87

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Cooling cream / Cooling cream with rose oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30889-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cooling cream / Cooling cream with rose oil; Cooling cream DAB; Cooling cream DAB 6 (stabilised, contains rose oil); Unguentum leniens; Unguentum leniens DAB 6

Special notes

When selecting the *Cooling cream / Cooling cream with rose oil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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 *Cooling cream / Cooling cream with rose oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cooling cream DAB	12364802	30889	120	20121217
Bombastus	Cooling cream DAB	275667	30890	80	20121221
Henry Lamotte	Cooling cream DAB	5321500	30921	80	20120627
Caelo	Cooling cream DAB	13051601	31052	40	20130221
Caelo	Cooling cream DAB	13315101	31224	70	20130925

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cooling cream DA...	13317001	31249	40	1405180
Caelo	Cooling cream DA...	14085901	31457	40	20140326
Caelo	Cooling cream DAB	14118002	31471	40	AR-14-FG-012400-01
Caelo	Cooling cream DA...	153029	31922	40	20150911*
Caelo	Cooling cream DAB	153277	31992	40	20150930*
Caelo	Cooling cream DA...	160896	32294	40	20160405*
Caelo	Cooling cream DA...	162223	32506	40	20160727*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 670 spectra of 12 reference samples from the substance/substance group *Cooling cream / Cooling cream with rose oil*. These samples are listed above in the [calibration samples](#) section.
- 33 674 spectra from a total of 786 batches from further 223 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 1512 spectra of 40 reference samples from the substance/substance group *Cooling cream / Cooling cream with rose oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cooling cream DAB	11107002	30324	42
Caelo	Cooling cream DAB	12001901	30464	30
Infectopharm	Cooling cream DAB 6 (stabili...	12003001	30585	40
Caelo	Cooling cream DAB	12364802	30889 [†]	10
Bombastus	Cooling cream DAB	275667	30890 [†]	10
Caelo	Cooling cream DAB 6 (stabili...	12306001	31037	40
Caelo	Cooling cream DAB 6 (stabili...	153029	31922 [†]	20
Caelo	Cooling cream DAB	153277	31992 [†]	20
Caelo	Cooling cream DAB	153281	31993	60
Caelo	Cooling cream DAB	161293	32227	40
Caelo	Cooling cream DAB	161293	32228	40

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

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cooling cream DAB	161294	32229	40
Caelo	Cooling cream DAB	161295	32230	40
Caelo	Cooling cream DAB	161296	32231	40
Caelo	Cooling cream DAB	161297	32232	40
Caelo	Cooling cream DAB	161341	32233	40
Caelo	Cooling cream DAB	161342	32234	40
Caelo	Cooling cream DAB	161338	32235	40
Caelo	Cooling cream DAB 6 (stabili...	160897	32293	40
Caelo	Cooling cream DAB	161718	32408	40
Caelo	Cooling cream DAB	161719	32409	40
Caelo	Cooling cream DAB	161719	32410	40
Caelo	Cooling cream DAB	161720	32411	40
Caelo	Cooling cream DAB	161720	32412	40
Caelo	Cooling cream DAB	161725	32413	40
Caelo	Cooling cream DAB	161727	32414	40
Caelo	Cooling cream DAB	161728	32415	40
Caelo	Cooling cream DAB	161729	32416	40
Caelo	Cooling cream DAB 6 (stabili...	162224	32507	40
Caelo	Cooling cream DAB	162445	32624	40
Caelo	Cooling cream DAB	162446	32625	40
Caelo	Cooling cream DAB	162447	32626	40
Caelo	Cooling cream DAB	162462	32627	40
Caelo	Cooling cream DAB	162463	32628	40
Caelo	Cooling cream DAB	162464	32629	40
Caelo	Cooling cream DAB	163017	32888	40
Caelo	Cooling cream DAB	163018	32889	40
Caelo	Cooling cream DAB	163019	32890	40
Caelo	Cooling cream DAB	163020	32891	40
Caelo	Cooling cream DAB	163021	32892	40

- 62082 spectra from a total of 1440 batches from further 438 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.

- 2153 spectra from 248 *Apo-Ident* customers from 744 batches from the substance/substance group *Cooling cream / Cooling cream with rose oil*.

Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB	12292401	4
Caelo	Cooling cream DAB	12364601	12
Caelo	Cooling cream DAB	12011402	1
Caelo	Cooling cream DAB	13051601	8
Caelo	Cooling cream DAB	12090401	3
Caelo	Cooling cream DAB	13059901	8

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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
Caelo	Cooling cream DAB	12312102	4
Phönix	Cooling cream DAB	13121001	3
Noweda	Cooling cream DAB	13121002	1
Caelo	Cooling cream DAB	13175101	7
Phönix	Cooling cream DAB	13121701	1
Caelo	Cooling cream DAB	13175201	7
Caelo	Cooling cream DAB	13191501	4
Caelo	Cooling cream DAB	13191801	7
Caelo	Cooling cream DAB	13191701	6
Phönix	Cooling cream DAB	13191801	1
Caelo	Cooling cream DAB	13192101	7
Caelo	Cooling cream DAB	13226501	9
Caelo	Cooling cream DAB	13191901	4
Caelo	Cooling cream DAB	13226801	17
Berkel AHK	Cooling cream DAB	13226301	3
Caelo	Cooling cream DAB	14000301	12
gehe 7.12.13	Cooling cream DAB	13226701	1
Phönix	Cooling cream DAB	13227401	1
Caelo	Cooling cream DAB	13402201	16
Caelo	Cooling cream DAB	13315101	24
Caelo	Cooling cream DAB	14055301	7
Caelo	Cooling cream DAB	14000401	2
Phönix	Cooling cream DAB	14055401	2
Caelo	Cooling cream DAB	14086301	8
Großhandel	Cooling cream DAB	14055501	1
Noweda	Cooling cream DAB	14085901	1
Caelo	Cooling cream DAB	14145701	5
Caelo	Cooling cream DAB	14271101	1
Caelo	Cooling cream DAB	14185101	5
Caelo	Cooling cream DAB	14145901	10
Caelo	Cooling cream DAB	14278201	8
Caelo	Cooling cream DAB	14278301	11
Caelo	Cooling cream DAB	16000801	4
Caelo	Cooling cream DAB	15435101	2
Caelo	Cooling cream DAB	16172601	8
Caelo	Cooling cream DAB	275666	3
Caelo	Cooling cream DAB	1915M-02541	1
Caelo	Cooling cream DAB	279753	1
Ginkgo-Apotheke	Cooling cream DAB	278439	1
Henry Lamotte/GEHE	Cooling cream DAB	5407300	1
Caelo	Cooling cream DAB	16129501	3
Lamotte/AHD	Cooling cream DAB	5600300	2
sanacorp/Lamotte	Cooling cream DAB	5735600	1
Henry Lamotte Oils/GEHE	Cooling cream DAB	5496200	1
Caelo	Cooling cream DAB	73/AKD3	1
lamotte/sanacorb	Cooling cream DAB	5496200	1
Sanacorp	Cooling cream DAB	73AKD4	1
Sanacorp	Cooling cream DAB	76/AKD3	1
Sanacorp	Cooling cream DAB		1
Caelo	Cooling cream DAB	14184801	4
Caelo	Cooling cream DAB	123test	2
Caelo	Cooling cream DAB	1256856	1
Caelo	Cooling cream DAB	15434501	7
Caelo	Cooling cream DAB	15434502	5
Caelo	Cooling cream DAB 6 (stabili...	15435101	1
Caelo	Cooling cream DAB	15435102	7
Caelo	Cooling cream DAB	16000201	2
Caelo	Cooling cream DAB	16000601	3
Phoenix	Cooling cream DAB 6 (stabili...	16000501	2
Caelo	Cooling cream DAB	16000501	1

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB	16085902	1
Caelo	Cooling cream DAB	16085801	4
Phoenix	Cooling cream DAB	16085801	1
Caelo	Cooling cream DAB 6 (stabili...	16085801	1
Phoenix	Cooling cream DAB	16086001	1
Caelo	Cooling cream DAB	16086001	1
Caelo	Cooling cream DAB	16129401	2
Caelo	Cooling cream DAB 6 (stabili...	16086001	1
Caelo	Cooling cream DAB	16086101	1
Caelo	Cooling cream DAB 6 (stabili...	16086101	1
Caelo	Cooling cream DAB 6 (stabili...	16129501	2
Euro OTC	Cooling cream DAB	16129501	1
Caelo	Cooling cream DAB	16129701	1
Caelo	Cooling cream DAB 6 (stabili...	16129701	2
Caelo	Cooling cream DAB	16134201	6
Caelo	Cooling cream DAB	16134001	2
Caelo	Cooling cream DAB	16129502	1
Caesar & Loretz/Noweda	Cooling cream DAB 6 (stabili...	16134201	1
Phoenix	Cooling cream DAB	16134001	1
Phoenix	Cooling cream DAB	16172001	1
Celo/ Kehr	Cooling cream DAB	16172001	1
Caelo	Cooling cream DAB 6 (stabili...	16172001	1
Caelo	Cooling cream DAB 6 (stabili...	16172601	3
Phoenix	Cooling cream DAB	16172701	1
Gehe	Cooling cream DAB	16244601	1
Caelo	Cooling cream DAB	16244701	2
Caelo	Cooling cream DAB 6 (stabili...	16172902	1
Caelo	Cooling cream DAB 6 (stabili...	16244701	1
Caelo	Cooling cream DAB	16172901	1
Bombastus	Cooling cream DAB	299351	1
Bombastus	Cooling cream DAB	300720	1
Bombastus	Cooling cream DAB	299967	1
Bombastus	Cooling cream DAB	300715	1
Bombastus	Cooling cream DAB	300730	2
Euro OTC	Cooling cream DAB	299976	1
Bombastus	Cooling cream DAB	299362	1
Bombastus	Cooling cream DAB	300727	1
Bombastus	Cooling cream DAB	301674	1
Bombastus	Cooling cream DAB	301700	1
Bombastus	Cooling cream DAB	301699	2
Ebert & Jacobi 02.08.16	Cooling cream DAB	301701	1
Bombastus	Cooling cream DAB	301701	2
Fagron	Cooling cream DAB	302370	2
Bombastus	Cooling cream DAB	302371	1
Bombastus	Cooling cream DAB	302385	1
Bombastus	Cooling cream DAB	302374	1
Bombastus	Cooling cream DAB	302372	1
Bombastus	Cooling cream DAB	303153	1
Bombastus	Cooling cream DAB	303625	1
Bombastus	Cooling cream DAB	304582	2
Bombastus	Cooling cream DAB	303621	1
Bomastus/Phönix	Cooling cream DAB	304582	1
Bombastus	Cooling cream DAB	305021	1
Bombastus	Cooling cream DAB	305022	1
Lamotte/AHD	Cooling cream DAB	6003682010	3
Caelo	Cooling cream DAB 6 (stabili...	15228501	3
Caelo	Cooling cream DAB 6 (stabili...	15237101	2
Caelo	Cooling cream DAB	15328001	13
Caelo	Cooling cream DAB	15417401	1
Caelo	Cooling cream DAB	15417501	4

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB	15434401	3
Alliance H.	Cooling cream DAB	15434401	1
Caesar & Loretz/Noweda	Cooling cream DAB 6 (stabili...	15328001	2
Caelo	Cooling cream DAB	15434402	3
Caelo	Cooling cream DAB 6 (stabili...	15434502	4
Caelo	Cooling cream DAB		4
Caelo	Cooling cream DAB	1543501	1
Caelo	Cooling cream DAB 6 (stabili...	15434503	1
Caelo	Cooling cream DAB	1543502	1
Phönix	Cooling cream DAB 6 (stabili...	15434502	1
Euro OTC	Cooling cream DAB	15435101	1
Caelo	Cooling cream DAB 6 (stabili...	15435102	1
Caelo	Cooling cream DAB 6 (stabili...	16000601	1
Noweda	Cooling cream DAB	16000801	1
Caelo	Cooling cream DAB 6 (stabili...	16089702	1
Caelo	Cooling cream DAB	16129601	1
Caelo	Cooling cream DAB	16133901	1
Caesar & Loretz/Noweda	Cooling cream DAB 6 (stabili...	16172601	1
Caelo	Cooling cream DAB	16134101	1
Caelo	Cooling cream DAB	16244601	1
Bombastus	Cooling cream DAB	299966	1
Caelo	Cooling cream DAB	5215A-02541	1
Caelo	Cooling cream DAB	17000301	1
Bombastus	Cooling cream DAB	265548	1
Bombastus	Cooling cream DAB	302382	1
Bombastus	Cooling cream DAB	298113	1
Bombastus	Cooling cream DAB	265549	1
Gehe	Cooling cream DAB	266839	2
Bombastus	Cooling cream DAB	265554	1
Bombastus	Cooling cream DAB	266941	1
Bombastus	Cooling cream DAB	268073	3
Bombastus	Cooling cream DAB	266717	1
Bombastus	Cooling cream DAB	268194	2
Phönix	Cooling cream DAB	268978	1
Bombastus	Cooling cream DAB	268981	1
Bombastus	Cooling cream DAB	269088	1
Gehe	Cooling cream DAB	269098	3
Gehe	Cooling cream DAB	269093	2
Bombastus	Cooling cream DAB	270309	1
Bombastus	Cooling cream DAB	271632	1
Caelo	Cooling cream DAB	1071408	1
Caelo	Cooling cream DAB	2091404	1
Gehe	Cooling cream DAB	271535	1
Caelo	Cooling cream DAB	1071407	1
Bombastus	Cooling cream DAB	270381	1
Caelo	Cooling cream DAB	4051503	2
Caelo	Cooling cream DAB	1097071	1
Caelo	Cooling cream DAB	4061203	1
Caelo	Cooling cream DAB	4061405	1
Caelo	Cooling cream DAB	8121403	1
Caelo	Cooling cream DAB	7071203	1
Caelo	Cooling cream DAB	5031509	1
Caesar & Loretz GmbH 40...	Cooling cream DAB	11299001	1
Caelo	Cooling cream DAB	11323101	2
Caelo	Cooling cream DAB	11268501	1
Caelo	Cooling cream DAB	11321402	1
Caelo	Cooling cream DAB	11322901	1
Caelo	Cooling cream DAB	11368201	1
Caelo	Cooling cream DAB	11368101	1
Caelo	Cooling cream DAB	12001901	3

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB	12002101	2
Caelo	Cooling cream DAB	12002501	3
Caelo	Cooling cream DAB	12002401	1
Caelo	Cooling cream DAB	12045901	1
Noweda	Cooling cream DAB	12045901	1
Fiebig ek: 9.07EUR	Cooling cream DAB	1204001	1
Caesar & Loretz GmbH, 4. .	Cooling cream DAB	12046201	2
Noweda	Cooling cream DAB	12046101	2
Noweda	Cooling cream DAB	12046201	1
Kehr	Cooling cream DAB	12046101	1
Caesar & Loretz GmbH, 4. .	Cooling cream DAB	12046001	1
Caelo	Cooling cream DAB	12051401	1
Caelo	Cooling cream DAB	12046401	1
Caelo	Cooling cream DAB	12051701	2
Caelo	Cooling cream DAB	12051402	1
Caelo	Cooling cream DAB	12089601	5
Caelo	Cooling cream DAB	12089701	1
Anzag 05.02.13 ek: 9,38EUR	Cooling cream DAB	12312801	1
Kehr	Cooling cream DAB	12089801	1
Caelo	Cooling cream DAB	120601202	1
Anzag 27.12.12 ek:9,09	Cooling cream DAB	12312301	1
DAB 2008	Cooling cream DAB	12089601	1
Caelo	Cooling cream DAB	12089901	1
Anzag 31.10.12 ek:9.12EUR	Cooling cream DAB	12187301	1
Caelo	Cooling cream DAB	13214010	1
Caelo	Cooling cream DAB	13175301	16
Caelo	Cooling cream DAB	1315601	1
Anzag 07.05.13 ek: 9,38EUR	Cooling cream DAB	13059701	1
Caelo	Cooling cream DAB	13226601	21
Caelo	Cooling cream DAB 6 (stabili. . .	1328702	1
Sanacorp	Cooling cream DAB	13227001	1
Caelo	Cooling cream DAB	13315201	6
Caelo	Cooling cream DAB	13315601	6
Caelo	Cooling cream DAB	13315701	2
Caelo	Cooling cream DAB	13315801	6
Caelo	Cooling cream DAB	13316001	1
Caelo	Cooling cream DAB	13401801	18
Caelo	Cooling cream DAB	13401901	6
Caelo	Cooling cream DAB	13402101	7
Caelo	Cooling cream DAB	14000101	2
Caelo	Cooling cream DAB	14000201	5
Caelo	Cooling cream DAB	14000501	5
Caelo	Cooling cream DAB	14028501	1
Großhandel	Cooling cream DAB	14055301	1
Großhandel	Cooling cream DAB	14055401	1
Caelo	Cooling cream DAB	14055401	1
Caelo	Cooling cream DAB	14055601	9
Caelo	Cooling cream DAB	14055702	6
Caelo	Cooling cream DAB	14071204	1
GEHE 14.04.2014	Cooling cream DAB	14055703	2
Caelo	Cooling cream DAB	14085901	12
Bombastus	Cooling cream DAB	14062101	1
Caesar & Loretz GmbH	Cooling cream DAB	14085901	2
Gehe	Cooling cream DAB	14085901	1
Caelo	Cooling cream DAB	14085902	4
Caelo	Cooling cream DAB	14086001	3
Phoenix 20.06.2014	Cooling cream DAB	14086001	1
Caelo	Cooling cream DAB	14086101	3
Caelo	Cooling cream DAB	14086201	3
Cealo	Cooling cream DAB	14086201	1

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB	1408631	1
Caelo	Cooling cream DAB	14086601	3
Caelo	Cooling cream DAB	14086401	2
Caelo	Cooling cream DAB	14086501	1
Caelo	Cooling cream DAB	14101401	1
Caelo	Cooling cream DAB	14086801	3
Caelo	Cooling cream DAB	14097214	1
Caelo	Cooling cream DAB	1412801	1
Caelo	Cooling cream DAB	14129401	11
Gehe	Cooling cream DAB	14129401	2
Gehe	Cooling cream DAB	14129402	1
Caelo	Cooling cream DAB	14129501	4
Caelo	Cooling cream DAB	14129402	2
Caelo	Cooling cream DAB	14129801	14
Noweda	Cooling cream DAB	14129801	2
Fagron	Cooling cream DAB	14132001	1
Caelo	Cooling cream DAB	14132201	4
Caelo	Cooling cream DAB	14132001	1
Caelo	Cooling cream DAB	14132301	7
Caelo	Cooling cream DAB	14132401	12
Caelo	Cooling cream DAB	14145501	12
Sanacorp	Cooling cream DAB	14145501	1
Caelo	Cooling cream DAB	14143101	1
Caelo	Cooling cream DAB	14145602	1
Caelo	Cooling cream DAB	14145801	4
Caelo	Cooling cream DAB	1418401	1
Caelo	Cooling cream DAB	14184301	1
Caelo	Cooling cream DAB	14184401	7
Caelo	Cooling cream DAB	14184501	5
Caelo	Cooling cream DAB	14184402	2
Caelo	Cooling cream DAB	14184601	14
Caesar & Loretz GmbH	Cooling cream DAB	14184501	1
Caelo	Cooling cream DAB	14184701	5
Caelo	Cooling cream DAB	14184901	4
Caelo	Cooling cream DAB	14185001	6
Caelo	Cooling cream DAB 6 (stabili...	14268101	2
Caelo	Cooling cream DAB	14200401	1
Caelo	Cooling cream DAB	14268101	6
Caelo	Cooling cream DAB	14186601	1
Berkel AHK	Cooling cream DAB	14268101	1
Caelo	Cooling cream DAB	14268301	10
Caelo	Cooling cream DAB	14271401	6
Caelo	Cooling cream DAB	14271201	2
DAB 2010	Cooling cream DAB	14269301	1
Allianz Healthcare 05.1...	Cooling cream DAB	14271101	1
Caelo	Cooling cream DAB 6 (stabili...	14271401	2
Caelo	Cooling cream DAB	14271501	3
Caelo	Cooling cream DAB	142728301	1
Caelo	Cooling cream DAB 6 (stabili...	14278301	2
Caelo	Cooling cream DAB	14278401	3
Caelo	Cooling cream DAB	14278502	4
Caelo	Cooling cream DAB	14278601	3
Caelo	Cooling cream DAB	14288601	5
Caesar & Loretz GmbH	Cooling cream DAB	14278701	1
Caelo	Cooling cream DAB 6 (stabili...	14288601	1
Caelo	Cooling cream DAB	14288701	4
Caelo	Cooling cream DAB	14288701	1
Caelo	Cooling cream DAB	14328701	1
Calo/AHD	Cooling cream DAB	14328702	1
Henry Lamotte	Cooling cream DAB	14328702	1

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB 6 (stabili. ...	14328702	2
Caelo	Cooling cream DAB	14328801	10
Caelo	Cooling cream DAB	14328702	2
Caelo	Cooling cream DAB 6 (stabili. ...	14328801	3
Sanacorp	Cooling cream DAB	14328801	2
Phönix	Cooling cream DAB	14328801	1
Caelo	Cooling cream DAB	14328901	3
Caelo	Cooling cream DAB	14329001	4
Caelo	Cooling cream DAB 6 (stabili. ...	14329001	1
Caelo	Cooling cream DAB	14329201	3
Caelo	Cooling cream DAB	14329401	5
Caelo	Cooling cream DAB	14329301	2
Caelo	Cooling cream DAB 6 (stabili. ...	14329401	1
phönix	Cooling cream DAB 6 (stabili. ...	14329501	1
Caelo	Cooling cream DAB	14329501	3
Gehe	Cooling cream DAB	14329501	1
Caelo	Cooling cream DAB	14329601	6
Caelo	Cooling cream DAB 6 (stabili. ...	14329601	1
Caelo/ Noweda	Cooling cream DAB	14c06-t02010890	1
Caelo	Cooling cream DAB	1468201	1
Phönix	Cooling cream DAB	14850901	1
Kremer/Phönix	Cooling cream DAB	15/158/K	1
Fagron	Cooling cream DAB	14A20	1
Caelo	Cooling cream DAB	15049201	13
Caelo	Cooling cream DAB	15049202	2
Caelo	Cooling cream DAB 6 (stabili. ...	15049202	2
Caelo	Cooling cream DAB	15052801	11
Caelo	Cooling cream DAB 6 (stabili. ...	15052801	1
Caelo	Cooling cream DAB	15053001	3
Caelo	Cooling cream DAB	15058801	4
Caelo	Cooling cream DAB	15058901	2
Caelo	Cooling cream DAB	15059001	2
Caelo	Cooling cream DAB 6 (stabili. ...	15059001	2
Caelo	Cooling cream DAB	15059201	8
Caelo	Cooling cream DAB	15066501	2
Caelo	Cooling cream DAB 6 (stabili. ...	15066601	2
Sanacorp	Cooling cream DAB	15066601	2
Caelo	Cooling cream DAB	15066601	5
Noweda	Cooling cream DAB	15066601	1
Caelo	Cooling cream DAB	15066701	2
Caelo	Cooling cream DAB	15066801	5
Caelo	Cooling cream DAB	15066801test	1
Caelo	Cooling cream DAB	15069201	1
Caelo	Cooling cream DAB	15066901	1
Caelo	Cooling cream DAB	15152801	2
Caelo	Cooling cream DAB	1513101	1
Caelo	Cooling cream DAB	15152901	2
Caelo	Cooling cream DAB	15153001	3
Caelo	Cooling cream DAB 6 (stabili. ...	15153101	1
Caelo	Cooling cream DAB 6 (stabili. ...	15153201	1
Caelo	Cooling cream DAB	15153101	2
Caelo	Cooling cream DAB	15153201	3
Caelo	Cooling cream DAB	15153301	1
Caelo	Cooling cream DAB 6 (stabili. ...	15153301	1
Caelo	Cooling cream DAB	15153202	1
Caelo	Cooling cream DAB	15153501	9
Caelo	Cooling cream DAB	15153401	1
Caelo	Cooling cream DAB 6 (stabili. ...	15153501	1
Caelo	Cooling cream DAB	15153701	5
Caelo	Cooling cream DAB 6 (stabili. ...	15228401	1

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB	15228401	2
Caelo	Cooling cream DAB	15228501	6
Caelo	Cooling cream DAB	15228601	19
Caelo	Cooling cream DAB 6 (stabili...	15228502	1
Cae/Phönix	Cooling cream DAB	15228601	1
Rondell Apotheke	Cooling cream DAB	15228601	1
Caelo	Cooling cream DAB 6 (stabili...	15228601	1
Caesar & Loretz GmbH	Cooling cream DAB	15228601	1
Caelo	Cooling cream DAB	15228701	5
Chiesi	Cooling cream DAB	15228701	1
Caelo	Cooling cream DAB	15228801	4
Caelo	Cooling cream DAB	15236701	1
Fagron	Cooling cream DAB	15236801	1
Caelo	Cooling cream DAB	15236801	1
Caelo	Cooling cream DAB 6 (stabili...	15236901	4
Caelo	Cooling cream DAB	15236901	8
Caelo	Cooling cream DAB	15237101	5
Caelo	Cooling cream DAB	15327701	4
Caelo	Cooling cream DAB	15327801	2
Caelo	Cooling cream DAB 6 (stabili...	15327901	1
Caelo	Cooling cream DAB	15327901	1
Caelo	Cooling cream DAB 6 (stabili...	15328001	4
Caelo	Cooling cream DAB	15413501	1
Caelo	Cooling cream DAB 6 (stabili...	15413601	1
Caelo	Cooling cream DAB	15413601	3
Caelo	Cooling cream DAB	15328101	2
Caelo	Cooling cream DAB	15413701	3
Caelo	Cooling cream DAB	15413901	1
Caelo	Cooling cream DAB 6 (stabili...	15413901	1
Caelo	Cooling cream DAB	15417201	5
Noweda	Cooling cream DAB	15417201	1
Caelo	Cooling cream DAB	15417601	2
Caesar & Loretz GmbH	Cooling cream DAB	15434401	1
Cordes/Phönix	Cooling cream DAB	15434402	1
Cealo/AHD	Cooling cream DAB	15434402	1
Caelo	Cooling cream DAB 6 (stabili...	15434501	5
Caelo	Cooling cream DAB	15434503	1
Caelo	Cooling cream DAB 6 (stabili...	16000201	1
Caelo	Cooling cream DAB	19051505	1
Caelo	Cooling cream DAB	23121412	1
Caelo	Cooling cream DAB	21071401	1
Caelo	Cooling cream DAB	16071505	1
Cealo/AHD	Cooling cream DAB 6 (stabili...	16011901	1
Caelo	Cooling cream DAB	27061201	1
Caelo	Cooling cream DAB	19051506	1
Bombastus	Cooling cream DAB	271726	1
Bombastus	Cooling cream DAB	2405212541	1
Bombastus	Cooling cream DAB	283119	1
Bombastus	Cooling cream DAB	284299	2
Caelo	Cooling cream DAB	283118	1
Bombastus	Cooling cream DAB	282021	2
Bombastus	Cooling cream DAB	284298	1
Bombastus	Cooling cream DAB	284264	1
Bombastus	Cooling cream DAB	284302	1
Bombastus	Cooling cream DAB	285068	2
Bombastus	Cooling cream DAB	284303	3
Bombastus	Cooling cream DAB	285065	1
Bombastus	Cooling cream DAB	285069	3
Bombastus	Cooling cream DAB	285498	1
Bombastus	Cooling cream DAB	285502	2

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Supplier	Substance	Batch	Spectra
gehe	Cooling cream DAB	285498	1
Bombastus	Cooling cream DAB	285503	1
Caelo	Cooling cream DAB	285504	2
Bombastus	Cooling cream DAB	285635	2
Bombastus	Cooling cream DAB	285634	2
Bombastus	Cooling cream DAB	285637	1
Bombastus	Cooling cream DAB	285645	1
Bombastus	Cooling cream DAB	285638	2
Bombastus	Cooling cream DAB	286562	1
Fontapharm/Phönix	Cooling cream DAB	286565	1
Bombastus	Cooling cream DAB	285644	1
Bombastus	Cooling cream DAB	285639	1
Gehe	Cooling cream DAB	286565	1
Bombastus	Cooling cream DAB	286648	1
Bombastus	Cooling cream DAB	286650	3
Bombastus	Cooling cream DAB	286653	1
Bombastus	Cooling cream DAB	286654	3
Bombastus	Cooling cream DAB	287485	2
Phönix	Cooling cream DAB	287486	1
Bombastus	Cooling cream DAB	287544	2
Caelo	Cooling cream DAB	287544	1
Bombastus	Cooling cream DAB	287539	1
Bombastus	Cooling cream DAB	287542	1
Bombastus	Cooling cream DAB	288109	2
Bombastus	Cooling cream DAB	288152	3
Bombastus	Cooling cream DAB	288112	2
Bombastus	Cooling cream DAB	288107	1
Gehe	Cooling cream DAB	289187	1
Bombastus	Cooling cream DAB	288159	1
Phönix	Cooling cream DAB	289188	1
Bombastus	Cooling cream DAB	289187	1
Bombastus	Cooling cream DAB	289188	2
Bombastus	Cooling cream DAB	289189	1
Bombastus	Cooling cream DAB	289191	3
Bombastus	Cooling cream DAB	289256	1
Bombastus	Cooling cream DAB	289260	3
Fagron	Cooling cream DAB	289253	2
Caelo	Cooling cream DAB	289265	1
Bombastus	Cooling cream DAB	290383	1
Bombastus	Cooling cream DAB	290483	2
Bombastus	Cooling cream DAB	290380	1
Bombastus	Cooling cream DAB	290396	1
Gehe	Cooling cream DAB	290485	1
Bombastus	Cooling cream DAB 6 (stabili...	290486	1
Bombastus	Cooling cream DAB	290487	1
Beiersdorf / E	Cooling cream DAB	290486	1
Bombastus	Cooling cream DAB	290490	1
Bombastus	Cooling cream DAB	29072015A	1
Caelo	Cooling cream DAB	29081509	1
Bombastus	Cooling cream DAB	291558	1
Bombastus	Cooling cream DAB	291555	1
Bombastus	Cooling cream DAB	291552	1
Bombastus	Cooling cream DAB	291620	2
Bombastus	Cooling cream DAB	291618	1
Bombastus	Cooling cream DAB	292102	1
Bombastus	Cooling cream DAB	292103	1
Bombastus	Cooling cream DAB	292106	3
Bombastus	Cooling cream DAB	292107	1
Bombastus	Cooling cream DAB	292930	2
Bombastus	Cooling cream DAB	292280	1

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Supplier	Substance	Batch	Spectra
Bombastus	Cooling cream DAB	292936	1
Bombastus	Cooling cream DAB	292994	1
Bombastus	Cooling cream DAB	292997	2
Bombastus	Cooling cream DAB	293616	2
Bombastus	Cooling cream DAB	293622	1
Caelo	Cooling cream DAB	293748	1
Bombastus	Cooling cream DAB	293621	3
Bombastus	Cooling cream DAB	293750	1
Bombastus	Cooling cream DAB	295021	1
Caelo	Cooling cream DAB	295123	1
Bombastus	Cooling cream DAB	295183	1
EB-Ho	Cooling cream DAB	295184	1
Bombastus	Cooling cream DAB 6 (stabili...	295191	1
Bombastus	Cooling cream DAB	295184	1
Bombastus	Cooling cream DAB	295185	1
Bombastus	Cooling cream DAB	295756	1
Bombastus	Cooling cream DAB	296312	1
Bombastus	Cooling cream DAB	296316	1
Bombastus	Cooling cream DAB	297097	2
Bombastus	Cooling cream DAB	297214	1
Bombastus	Cooling cream DAB	297211	1
Bombastus	Cooling cream DAB	298118	1
Bombastus	Cooling cream DAB	297205	1
Bombastus	Cooling cream DAB	297206	1
Caelo	Cooling cream DAB	295762	1
Bombastus	Cooling cream DAB	298119	1
Bombastus	Cooling cream DAB	298121	1
Bombastus	Cooling cream DAB 6 (stabili...	298319	1
apomix Fiebig	Cooling cream DAB	299362	1
Bombastus	Cooling cream DAB	298881	1
Bombastus	Cooling cream DAB	299361	1
Henry Lamotte/GEHE	Cooling cream DAB	5163700	1
Caelo	Cooling cream DAB	30011505	1
Bombastus	Cooling cream DAB	299973	1
Caelo	Cooling cream DAB	3012M-02541	1
PHOENIX am 06.06.2012	Cooling cream DAB	5163800	1
Caelo	Cooling cream DAB	30091402	1
Lamotte Sanacorp	Cooling cream DAB	5496200	3
Lamotte Sanacorp	Cooling cream DAB	5600300	1
Lamotte/ Phönix	Cooling cream DAB	5600300	1
Henry Lamotte Oils/GEHE	Cooling cream DAB	5600300	1
Henry Lamotte Olis GmbH...	Cooling cream DAB	5600300	2
Henry Lamotte Olis GmbH	Cooling cream DAB	5735600	1
Henry Lamotte Oils/GEHE	Cooling cream DAB	5691200	1
Caelo	Cooling cream DAB	5735600	1
Henry Lamotte Oils/GEHE	Cooling cream DAB	5735600	1
Anzag	Cooling cream DAB	6002062002	1
Sanacorp/Henry Lamotte	Cooling cream DAB	6000083005	1
Sanacorp	Cooling cream DAB	77/AKD6	1
Bombastus	Cooling cream DAB	91709	1
Fagron	Cooling cream DAB	B15A30T07018676	1
Lamotte/AHD	Cooling cream DAB	6001092001	1
Phoenix	Cooling cream DAB	269094	1
Bombastus	Cooling cream DAB	269092	1
Gehe	Cooling cream DAB	270314	1
Bombastus	Cooling cream DAB	270315	1
Bombastus	Cooling cream DAB	271541	1
Bombastus	Cooling cream DAB	271623	1
Phönix	Cooling cream DAB	271541	1
Phoenix 12.11.12	Cooling cream DAB	271623	1

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Supplier	Substance	Batch	Spectra
Bombastus	Cooling cream DAB	271624	1
Bombastus	Cooling cream DAB	272349	1
Caelo	Cooling cream DAB	271631	1
Bombastus	Cooling cream DAB	271627	1
Bombastus	Cooling cream DAB	272353	1
Bombastus	Cooling cream DAB	272482	1
Anzag 25.10.12	Cooling cream DAB	272484	1
Caelo	Cooling cream DAB	272479	2
Bombastus	Cooling cream DAB	272485	1
Anzag, 25.10.2012	Cooling cream DAB	272486	1
Bombastus	Cooling cream DAB	272564	2
Bombastus	Cooling cream DAB	272572	2
Bombastus	Cooling cream DAB	273444	1
Anzag/	Cooling cream DAB	273441	3
Bombastus	Cooling cream DAB	273443	1
Bombastus	Cooling cream DAB	272573	2
Bombastus	Cooling cream DAB	273501	1
Bombastus	Cooling cream DAB	273499	1
Bombastus	Cooling cream DAB	274044	2
Gehe	Cooling cream DAB	274044	2
Bombastus	Cooling cream DAB	273503	1
ANZAG	Cooling cream DAB	273504	1
Noweda	Cooling cream DAB	274043	1
Sanacorp	Cooling cream DAB	274077	1
Bombastus	Cooling cream DAB	274083	2
Bombastus	Cooling cream DAB	274079	1
Bombastus	Cooling cream DAB	274077	1
Bombastus	Cooling cream DAB	274080	2
Bombastus	Cooling cream DAB	513A-02541	1
Caelo	Cooling cream DAB	2081201	1
Caelo	Cooling cream DAB	6111201	1
Caelo	Cooling cream DAB	6061303	1
Caelo	Cooling cream DAB	613I-02541	1
Caelo	Cooling cream DAB	6111202	1
Caelo	Cooling cream DAB	7021301	1
Bombastus	Cooling cream DAB	614U2541	1
Caelo	Cooling cream DAB	7091201	1
Caelo	Cooling cream DAB	8041304	1
Caelo	Cooling cream DAB	8111201	1
Caelo	Cooling cream DAB	913I-02541	1
Bombastus	Cooling cream DAB	1109212541	1
Caelo	Cooling cream DAB	10081209	1
Caelo	Cooling cream DAB	10081210	1
Caelo	Cooling cream DAB	10091306	1
Caelo	Cooling cream DAB	1113Q-02541	1
Caelo	Cooling cream DAB	11269101	1
Caelo	Cooling cream DAB	12052001	1
Caelo/Gehe	Cooling cream DAB	12052002	2
Caelo	Cooling cream DAB	12089301	2
Caelo	Cooling cream DAB	120522/1	1
Caelo	Cooling cream DAB	12089201	1
Caelo	Cooling cream DAB	12089401	1
Caelo	Cooling cream DAB	12089402	2
Phönix Gotha	Cooling cream DAB	12089501	1
Caelo	Cooling cream DAB	12090201	3
Phoenix, 04.09.2012	Cooling cream DAB	12090601	2
VDL	Cooling cream DAB	12090501	1
Caelo	Cooling cream DAB	12090501	2
Caelo	Cooling cream DAB	1213M-02541	2
Caelo	Cooling cream DAB	12090601	1

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Supplier	Substance	Batch	Spectra
Noweda	Cooling cream DAB	12174301	3
Caelo	Cooling cream DAB	12174301	2
Caesar & Loretz GmbH, 4...	Cooling cream DAB	12174401	2
Caelo	Cooling cream DAB	12174401	4
Caelo	Cooling cream DAB	12174501	1
Caelo	Cooling cream DAB	12174601	2
Caelo	Cooling cream DAB	12178801	2
Phönix, 30.10.2012	Cooling cream DAB	12178801	1
Caesar & Loretz GmbH	Cooling cream DAB	12178901	1
Caelo	Cooling cream DAB	12178902	3
Caelo	Cooling cream DAB	12178901	1
Großhandel	Cooling cream DAB	12178902	1
Caelo	Cooling cream DAB	12182701	5
Caelo	Cooling cream DAB	12179001	3
Erika apotheke	Cooling cream DAB	12182701	1
Caelo	Cooling cream DAB	12182801	3
Caesar & Loretz GmbH, 4...	Cooling cream DAB	12182801	2
Caelo	Cooling cream DAB	12187301	4
Caelo	Cooling cream DAB	12187201	3
Kehr	Cooling cream DAB	12187301	1
Phönix 26.10.12	Cooling cream DAB	12187301	1
Caelo	Cooling cream DAB	12253001	3
Caesar & Loretz GmbH D-...	Cooling cream DAB	12253001	1
Caelo	Cooling cream DAB	12253101	4
Großhandel	Cooling cream DAB	12253201	1
Caelo	Cooling cream DAB	12253201	3
Caelo	Cooling cream DAB	12253301	2
Caelo	Cooling cream DAB	12253401	2
Caelo	Cooling cream DAB	12290102	1
Caelo	Cooling cream DAB	12292102	17
Caelo	Cooling cream DAB	12291901	2
Caelo	Cooling cream DAB	12291301	2
Anzag 21.02.2013	Cooling cream DAB	12291901	1
Caelo	Cooling cream DAB	12292201	6
Phoenix 28.11.12	Cooling cream DAB	12292201	2
Großhandel	Cooling cream DAB	12292201	1
phönix	Cooling cream DAB	12292201	1
Caelo	Cooling cream DAB	12292301	8
Caesar & Loretz GmbH, 4...	Cooling cream DAB	12292301	1
Noweda	Cooling cream DAB	12292301	1
Gehe	Cooling cream DAB	12292401	1
Caesar & Loretz GmbH	Cooling cream DAB	12306001	1
Kehr	Cooling cream DAB	12312002	1
Caelo	Cooling cream DAB	12312101	2
phönix	Cooling cream DAB	12312102	1
Caelo	Cooling cream DAB	12312201	5
Caelo	Cooling cream DAB	12312301	1
Caelo	Cooling cream DAB	12312401	9
Caelo	Cooling cream DAB	12312501	3
Caelo	Cooling cream DAB	12312601	3
Caelo	Cooling cream DAB	12312701	3
Caelo	Cooling cream DAB	12312801	3
Sanacorp	Cooling cream DAB	12312801	1
Großhandel	Cooling cream DAB	12312801	1
Gehe	Cooling cream DAB	12312801	1
Caelo	Cooling cream DAB	12364701	2
Caelo	Cooling cream DAB	12364801	3
Caelo	Cooling cream DAB	12364802	1
GEHE	Cooling cream DAB	12364801	1
Caelo	Cooling cream DAB	1289501	1

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB	13004101	5
Noweda	Cooling cream DAB	12992301	1
Caelo	Cooling cream DAB	1290301	1
Caelo	Cooling cream DAB	1287201	1
Fagron	Cooling cream DAB	12G25-T02	2
Caelo	Cooling cream DAB	13004201	7
Caelo	Cooling cream DAB	13004401	3
cael	Cooling cream DAB	13004201	1
Caelo	Cooling cream DAB	13004301	3
Caelo	Cooling cream DAB	13004402	6
Kehr	Cooling cream DAB	13004501	1
Caelo	Cooling cream DAB	13004501	6
Caelo	Cooling cream DAB	13004601	4
Großhandel	Cooling cream DAB	13004601	1
Gehe	Cooling cream DAB	13004701	1
calo	Cooling cream DAB	13004701	2
Caelo	Cooling cream DAB	13026201	1
Caelo	Cooling cream DAB	13051401	5
Caelo	Cooling cream DAB	13047201	1
Caelo	Cooling cream DAB	13051501	8
Noweda	Cooling cream DAB	13051501	1
Caelo	Cooling cream DAB	13051602	4
Phönix	Cooling cream DAB	13051602	1
Caelo	Cooling cream DAB	13059501	2
Phönix	Cooling cream DAB	13059501	1
Großhandel	Cooling cream DAB	13059501	1
Caelo	Cooling cream DAB	13059601	9
Sanacorp	Cooling cream DAB	13059601	1
Großhandel	Cooling cream DAB	13059601	1
Caesar & Loretz GmbH, 4. .	Cooling cream DAB	13059601	1
Caelo	Cooling cream DAB	13059701	7
Phönix	Cooling cream DAB	13059901	1
Caelo	Cooling cream DAB	13059902	3
Caelo	Cooling cream DAB	13120901	14
Caelo	Cooling cream DAB	13068101	3
Caelo	Cooling cream DAB	13121001	9
Caelo	Cooling cream DAB	13121002	3
Lamotte/Phönix	Cooling cream DAB	1312101	3
Caelo	Cooling cream DAB	13121201	7
Caelo	Cooling cream DAB	13121301	5
Caesar & Loretz GmbH, 4. .	Cooling cream DAB	13121401	2
Caelo	Cooling cream DAB	13121401	9
Caelo	Cooling cream DAB	13121701	7
Caelo	Cooling cream DAB	13121501	1
Caelo	Cooling cream DAB	13121601	2
Caelo	Cooling cream DAB	13121503	1
Caesar & Loretz GmbH, 4. .	Cooling cream DAB	13121701	2
Großhandel	Cooling cream DAB	13121701	1
Anzag	Cooling cream DAB	13175101	1
Caelo	Cooling cream DAB	13175001	2
Caelo	Cooling cream DAB	1312601	1
Caesar & Loretz GmbH, 4. .	Cooling cream DAB	13175101	4
Caelo	Cooling cream DAB	13174901	1
Caelo	Cooling cream DAB	13191301	2
Caelo	Cooling cream DAB	13191401	10
Gehe	Cooling cream DAB	13191501	1
Großhandel	Cooling cream DAB	13191501	1
Caelo	Cooling cream DAB	13191601	6
Großhandel	Cooling cream DAB	13191801	1
Maros/Phoenix	Cooling cream DAB	13191901	1

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB	13192001	7
Caesar & Loretz GmbH, 4...	Cooling cream DAB	13192001	1
Phönix	Cooling cream DAB	13192101	1
Sanacorp	Cooling cream DAB	13192101	1
Caelo	Cooling cream DAB	13226301	7
Caelo	Cooling cream DAB	13192201	1
Caelo	Cooling cream DAB	1322601	1
Caelo	Cooling cream DAB	13225701	2
Caelo	Cooling cream DAB	13225801	1
AHD, 08.11.13	Cooling cream DAB	13225801	1
Caelo	Cooling cream DAB	13207201	1
Caelo	Cooling cream DAB	13226302	5
Phönix	Cooling cream DAB	13226302	1
Sanacorp	Cooling cream DAB	13226501	1
Caelo	Cooling cream DAB	13226602	1
Caelo	Cooling cream DAB	13226701	4
Sanacorp	Cooling cream DAB	13226701	1
Caelo	Cooling cream DAB	13226901	7
Caelo	Cooling cream DAB	13227001	3
Großhandel	Cooling cream DAB	13227001	3
Caelo	Cooling cream DAB	13227101	6
Gehe am 03.02.2014	Cooling cream DAB	1322701	1
Euro OTC	Cooling cream DAB	13227101	1
Caelo	Cooling cream DAB	13227201	8
Caelo	Cooling cream DAB	13227301	3
Caelo	Cooling cream DAB	13227401	8
Bombastus	Cooling cream DAB	13315101	2
Noweda	Cooling cream DAB	13315101	1
Caesar & Loretz GmbH	Cooling cream DAB	13315101	1
Caelo	Cooling cream DAB	13315102	3
gehe	Cooling cream DAB	13315102	1
Gehe	Cooling cream DAB	13315201	1
Caesar & Loretz GmbH	Cooling cream DAB	13315201	1
Caelo	Cooling cream DAB	13315401	1
Bombastus	Cooling cream DAB	13315701	1
Caesar & Loretz GmbH, 4...	Cooling cream DAB	13315601	1
Caelo	Cooling cream DAB	13315901	1
Caelo	Cooling cream DAB	133227401	1
Caelo	Cooling cream DAB	13327101	1
Sanacorp	Cooling cream DAB	13401801	1
Caelo	Cooling cream DAB	13402001	5
Sanacorp	Cooling cream DAB	13402001	1
Fagron	Cooling cream DAB	13D19-T01-002941	1
Fagron	Cooling cream DAB	13E10-T01-003539	2
Caelo	Cooling cream DAB	14055703	1
Caelo	Cooling cream DAB	14268201	1
Caelo	Cooling cream DAB	15011304	1
Caelo	Cooling cream DAB	1543512	1
Fagron	Cooling cream DAB	15A30-T07-018974	1
Caelo	Cooling cream DAB	16081303	1
Caelo	Cooling cream DAB	16101201	1
Caelo	Cooling cream DAB	17121301	1
Caelo	Cooling cream DAB	18121205	1
Caelo	Cooling cream DAB	22021305	1
Bombastus	Cooling cream DAB	2112212541	1
Caelo	Cooling cream DAB	22051307	1
Bombastus	Cooling cream DAB	2413Q02541	1
Caelo	Cooling cream DAB	25091308	1
Bombastus	Cooling cream DAB	2713Q2541	1
Bombastus	Cooling cream DAB	22487	1

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB	26071307	1
Caelo	Cooling cream DAB	27111201	1
Caelo	Cooling cream DAB	22061301	1
Bombastus	Cooling cream DAB	274042	1
Bombastus	Cooling cream DAB	272571	1
Gehe	Cooling cream DAB	274084	1
Caelo	Cooling cream DAB	25021414	1
Bombastus	Cooling cream DAB	274791	2
Bombastus	Cooling cream DAB	274785	1
Gehe	Cooling cream DAB	274909	2
Bombastus	Cooling cream DAB	275663	1
Bombastus	Cooling cream DAB	274914	1
Anzag	Cooling cream DAB	274911	1
Bombastus	Cooling cream DAB	275664	1
Bombastus	Cooling cream DAB	275668	1
Bombastus	Cooling cream DAB	275670	1
Bombastus	Cooling cream DAB	276281	1
Bombastus	Cooling cream DAB	276282	1
Gehe	Cooling cream DAB	276283	3
Bombastus	Cooling cream DAB	276288	1
Noweda	Cooling cream DAB	276284	1
Bombastus	Cooling cream DAB	276418	4
Bombastus	Cooling cream DAB	276284	1
Bombastus	Cooling cream DAB	276419	2
Bombastus	Cooling cream DAB	276422	2
Bombastus	Cooling cream DAB	277275	2
Bombastus	Cooling cream DAB	277363	1
Alliance Healthcare	Cooling cream DAB	277366	1
Alliance Healthcare	Cooling cream DAB	277368	1
Bombastus	Cooling cream DAB	277371	1
Bombastus	Cooling cream DAB	277525	2
Bombastus	Cooling cream DAB	277526	1
Bombastus	Cooling cream DAB	277530	2
Bombastus	Cooling cream DAB	277533	1
Fagron	Cooling cream DAB	277533	1
Alliance Healthcare	Cooling cream DAB	277534	1
Bombastus	Cooling cream DAB	277534	2
Bombastus	Cooling cream DAB	278337	1
Bombastus	Cooling cream DAB	278338	1
Bombastus	Cooling cream DAB	278342	1
Bombastus	Cooling cream DAB	278436	1
Bombastus	Cooling cream DAB	278439	2
Bombastus	Cooling cream DAB	278437	2
Bombastus	Cooling cream DAB	278440	3
Alliance Healthcare	Cooling cream DAB	278444	1
Bombastus	Cooling cream DAB	278441	1
Phönix	Cooling cream DAB	278516	2
Gehe	Cooling cream DAB	278518	1
Bombastus	Cooling cream DAB	278674	1
Alliance Healthcare	Cooling cream DAB	278523	1
Bombastus	Cooling cream DAB	279681	1
Bombastus	Cooling cream DAB	278525	2
Bombastus	Cooling cream DAB	279680	2
Gehe	Cooling cream DAB	279681	2
Bombastus	Cooling cream DAB	279682	2
Bombastus	Cooling cream DAB	279750	2
Bombastus	Cooling cream DAB	279755	3
Bombastus	Cooling cream DAB	279751	1
Bombastus	Cooling cream DAB	279765	2
Bombastus	Cooling cream DAB	279766	1

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB	28101302	1
Caelo	Cooling cream DAB	28021306	1
Bombastus	Cooling cream DAB	281030	1
Bombastus	Cooling cream DAB	281033	1
Bombastus	Cooling cream DAB	281134	1
Gehe	Cooling cream DAB	281036	1
Sanacorp	Cooling cream DAB	281037	1
Bombastus	Cooling cream DAB	281139	3
Bombastus	Cooling cream DAB	281140	1
Bombastus	Cooling cream DAB	281820	1
Caelo	Cooling cream DAB	28121203	1
Bombastus	Cooling cream DAB	281822	3
Bombastus	Cooling cream DAB	281824	1
Bombastus	Cooling cream DAB	281912	1
Bombastus	Cooling cream DAB	281919	1
Bombastus	Cooling cream DAB	282017	1
Caesar & Loretz GmbH	Cooling cream DAB	282019	1
Gehe	Cooling cream DAB	282020	1
Bombastus	Cooling cream DAB	282019	2
Caelo	Cooling cream DAB	282020	1
Gehe	Cooling cream DAB	282022	1
Gehe	Cooling cream DAB	283053	1
Bombastus	Cooling cream DAB	283058	1
Bombastus	Cooling cream DAB	283051	1
Bombastus	Cooling cream DAB	283057	1
Bombastus	Cooling cream DAB	283054	1
Bombastus	Cooling cream DAB	283116	1
Gehe	Cooling cream DAB	283114	1
Bombastus	Cooling cream DAB	283117	1
Bombastus	Cooling cream DAB	283118	1
Gehe	Cooling cream DAB	284300	1
Bombastus	Cooling cream DAB	284263	1
Bombastus	Cooling cream DAB	286652	1
Bombastus	Cooling cream DAB	284300	3
Euro OTC	Cooling cream DAB	286563	1
Gehe	Cooling cream DAB	285066	1
Caelo	Cooling cream DAB	30081302	1
Caelo	Cooling cream DAB	3413E-02541	1
Caelo	Cooling cream DAB	31011301	1
Caelo	Cooling cream DAB	4313I-02541	1
Anzag/	Cooling cream DAB	5316800	1
phönix 17.1.13	Cooling cream DAB	5316900	1
Bombastus	Cooling cream DAB	4013Q2541	1
Caelo	Cooling cream DAB	5132	1
Noweda/Lamotte Oils	Cooling cream DAB	5321500	1
Henry Lamotte/GEHE	Cooling cream DAB	5321500	1
Henry Lamotte	Cooling cream DAB	5321500	1
Henry Lamotte/GEHE	Cooling cream DAB	5316800	1
Caelo	Cooling cream DAB	5321500	1
Henry Lamotte	Cooling cream DAB	5407300	2
Henry Lamotte Oils/GEHE	Cooling cream DAB	5407600	1
Anzag/Lamotte	Cooling cream DAB	5407300	1
Lamotte/Anzag	Cooling cream DAB	5496200	2
Henry Lamotte	Cooling cream DAB	5496300	1
Bombastus	Cooling cream DAB	60082801	1
Bombastus	Cooling cream DAB	60082802	1
Caelo	Cooling cream DAB	72/AD2	1
Bombastus	Cooling cream DAB	77309	1
Phönix Gotha	Cooling cream DAB	SRTM1104	1
Bombastus	Cooling cream DAB	92086	1

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Supplier	Substance	Batch	Spectra
Caelo	Cooling cream DAB 6 (stabili. ...)	213E-02541	1
Caelo	Cooling cream DAB 6 (stabili. ...)	12182701	2
Euro OTC	Cooling cream DAB	caelo	1
Caelo	Cooling cream DAB 6 (stabili. ...)	12179001	1
Caelo	Cooling cream DAB 6 (stabili. ...)	12312701	1
Gehe	Cooling cream DAB 6 (stabili. ...)	12312601	1
Caelo	Cooling cream DAB 6 (stabili. ...)	12364802	1
Noweda	Cooling cream DAB 6 (stabili. ...)	13026301	2
Caelo	Cooling cream DAB 6 (stabili. ...)	13120901	3
Caelo	Cooling cream DAB 6 (stabili. ...)	13192101	3
Caelo	Cooling cream DAB 6 (stabili. ...)	13191901	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13175101	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13121401	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13047201	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13051401	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13051501	2
Caelo	Cooling cream DAB 6 (stabili. ...)	13175301	3
Caelo	Cooling cream DAB 6 (stabili. ...)	20130912-3	1
Gehe	Cooling cream DAB 6 (stabili. ...)	273502	1
Gehe	Cooling cream DAB 6 (stabili. ...)	12003002	1
Caelo	Cooling cream DAB 6 (stabili. ...)	12206101	1
Caelo	Cooling cream DAB 6 (stabili. ...)	1302601	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13004401	1
anzag, 21.01.2013	Cooling cream DAB 6 (stabili. ...)	12312301	1
Caelo	Cooling cream DAB 6 (stabili. ...)	12312501	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13051601	2
Caelo	Cooling cream DAB 6 (stabili. ...)	12312401	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13092901	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13121201	4
Sanacorp	Cooling cream DAB 6 (stabili. ...)	13121601	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13121701	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13174901	1
gehe 14.08.2013	Cooling cream DAB 6 (stabili. ...)	13191401	1
Sanacorp	Cooling cream DAB 6 (stabili. ...)	13191301	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13191501	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13191701	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13192001	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13226302	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13226601	2
Caelo	Cooling cream DAB 6 (stabili. ...)	14129801	1
Caelo	Cooling cream DAB 6 (stabili. ...)	13226801	1
Caelo	Cooling cream DAB 6 (stabili. ...)	14085901	1
Caelo	Cooling cream DAB 6 (stabili. ...)	14184601	1
Caelo	Cooling cream DAB	14268002	1
Caelo	Cooling cream DAB	16000401	1
Caelo	Cooling cream DAB	16085901	1
Caelo	Cooling cream DAB	16172801	1
Caelo	Cooling cream DAB	16246201	1
Caelo	Cooling cream DAB	16246301	1
Bombastus	Cooling cream DAB	285499	2
Bombastus	Cooling cream DAB	289265	1
Bombastus	Cooling cream DAB	291619	1
Bombastus	Cooling cream DAB	295124	1
Lamotte/Spangro	Cooling cream DAB	5735700	1
Lamotte/Spangro	Cooling cream DAB	5861100	12
Lamotte/Spangro	Cooling cream DAB	6000744001	3
Lamotte/Spangro	Cooling cream DAB	6001092002	5
Gutenberg-Apotheke	Cooling cream DAB	84187	1
Caelo	Cooling cream DAB	P158/14	1
Bombastus	Cooling cream DAB	270310	1

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Supplier	Substance	Batch	Spectra
Anzag	Cooling cream DAB	272348	1
Caelo	Cooling cream DAB	11323501	1
Sanacorp	Cooling cream DAB	13004401	2
Caelo	Cooling cream DAB	12312001	1
Sanacorp	Cooling cream DAB	13121001	1
A.H.D.	Cooling cream DAB	13226301	1
Caleo/Phönix	Cooling cream DAB	14086501	1
Anzag	Cooling cream DAB	272347	1
Anzag	Cooling cream DAB	274042	1
Bombastus	Cooling cream DAB	275665	1
Bombastus	Cooling cream DAB	274783	1
Bomba/AHD	Cooling cream DAB	277269	1
Bombastus	Cooling cream DAB	277367	1
Bombastus	Cooling cream DAB	277369	1
Bomba	Cooling cream DAB	278341	2
Bombastus	Cooling cream DAB	278335	3
Bombastus	Cooling cream DAB	278438	1
Bombastus	Cooling cream DAB	278442	1
Pharmachem/AHD	Cooling cream DAB	279680	1
Bombastus	Cooling cream DAB	279676	2
Bomba/AHD	Cooling cream DAB	281031	2
Caelo	Cooling cream DAB	281140	1
Bombastus	Cooling cream DAB	281823	1
Bomba/AHD	Cooling cream DAB	281920	1
ichthyol/AHD	Cooling cream DAB	281921	2
Bombastus	Cooling cream DAB	284265	1
Bomba/AHD	Cooling cream DAB	283115	1
Anzag	Cooling cream DAB	60082802	1
Anzag	Cooling cream DAB	5253700	1
Gehe	Cooling cream DAB 6 (stabili...	14268301	1
Gehe	Cooling cream DAB 6 (stabili...	14184501	1
Henry Lamotte/N/19.11.12	Cooling cream DAB	5253700	1

- 56 288 spectra from 331 *Apo-Ident* customers from a total of 19 363 batches from a further 327 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 *Cooling cream / Cooling cream with rose 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 *Cooling cream / Cooling cream with rose 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	670	0	33 674
Type B	0	1482	30	62 082
Type C	0	2099	54	56 288

The substance/substance group *Cooling cream / Cooling cream with rose 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 % (> 99.9689 %)	100.0000 % (> 99.1045 %)
Type B	100.0000 % (> 99.9710 %)	98.0159 % (> 97.8175 %)
Type C	100.0000 % (> 99.5963 %)	97.4919 % (> 97.3525 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30889	31992	8.26	35.28
30890	31249	9.79	46.72
30921	31249	5.04	40.93
31052	31922	6.81	38.14
31224	31992	7.38	38.55
31249	31249	0.00	41.96
31457	31992	11.94	36.04
31471	31471	0.00	35.76
31922	31922	0.00	41.08
31992	31992	0.00	39.92
32294	32294	0.00	34.58
32506	32506	0.00	43.48

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Cordesian shaking mixture
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31075-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cordesian shaking mixture; Cordes lotio

Special notes

When selecting the *Cordesian shaking mixture* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Cordesian shaking mixture*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Ichthyol	Cordesian shakin...	12D014	31075	40	1403759
Ichthyol	Cordesian shakin...	14D010	31595	20	20140826
Ichthyol	Cordesian shakin...	15D002	32487	40	20150318

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Cordesian shaking mixture*. These samples are listed above in the [calibration samples](#) section.
- 34 244 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Cordesian shaking mixture*.

Supplier	Substance	Batch	Sample ID	Spectra
Ichthyol	Cordesian shaking mixture	11D029	30505	40
Ichthyol	Cordesian shaking mixture	14D010	31595 [†]	40

- 63 514 spectra from a total of 1475 batches from further 439 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.

- 40 spectra from 15 *Apo-Ident* customers from 14 batches from the substance/substance group *Cordesian shaking mixture*.

Supplier	Substance	Batch	Spectra
Ichthyol/Phönix	Cordesian shaking mixture	14D011	3
Ichthyol/Phönix	Cordesian shaking mixture	15D001	2

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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
Ichthyol/Phönix	Cordesian shaking mixture	15D002	2
Anzag/Ichthyol-Gesellsch...	Cordesian shaking mixture	13D009	1
Ichthyol	Cordesian shaking mixture	11D030	1
Caelo	Cordesian shaking mixture	12081403	1
Ichthyol	Cordesian shaking mixture	13D009	1
Ichthyol-Gesellschaft, ...	Cordesian shaking mixture	13D010	1
Alliance Health 05.06.2...	Cordesian shaking mixture	11D029	1
Ichthyol	Cordesian shaking mixture	13D010	1
Ichthyol / Noweda	Cordesian shaking mixture	14D010	2
Ichthyol	Cordesian shaking mixture	14041402	1
Ichthyol/gehe	Cordesian shaking mixture	14D010	2
Ichthyol/Sanacorp	Cordesian shaking mixture	14D010	1
Ichthyol/Phoenix	Cordesian shaking mixture	14D010	1
Ichthyol	Cordesian shaking mixture	14D010	2
Ichthyol /Noweda	Cordesian shaking mixture	15D001	1
Ichthyol	Cordesian shaking mixture	14D011	1
Ichthyol	Cordesian shaking mixture	15D001	2
Ichthyol/Anzag	Cordesian shaking mixture	15D002	1
Ichthyol-Gesellschaft	Cordesian shaking mixture	15D001	1
Ichthyol/Phoenix	Cordesian shaking mixture	15D002	1
Ichthyol	Cordesian shaking mixture	15D002	2
ichthyol	Cordesian shaking mixture	12D014	1
Ichthyol	Cordesian shaking mixture	16021509	1
Ichthyol	Cordesian shaking mixture	27041508	1
Ichthyol	Cordesian shaking mixture	27041507	1
Ichthyol/Phönix	Cordesian shaking mixture	13D009	1
Phoenix/Stiefel	Cordesian shaking mixture	12D014	1
Caelo	Cordesian shaking mixture	15D002	1
Ichthyol/gehe	Cordesian shaking mixture	13D010	1

- 58 401 spectra from 332 *Apo-Ident* customers from a total of 20 078 batches from a further 328 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 *Cordesian shaking mixture* 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 *Cordesian shaking mixture* 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	34 244
Type B	0	80	0	63 514
Type C	0	40	0	58 376

The substance/substance group *Cordesian shaking mixture* 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 % (> 99.9691 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5966 %)	100.0000 % (> 85.0000 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31075	31075	0.00	30.15
31595	31075	3.94	29.25
32487	31075	6.94	37.69

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Coriander oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31192-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Coriander oil; Oleum coriandri

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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 *Coriander oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Coriander oil	12228509	31192	40	1407274
Caelo	Coriander oil	13288109	31407	40	20130903

Validation samples

A total of 156 379 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 *Coriander oil*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 121 spectra of 3 reference samples from the substance/substance group *Coriander oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Coriander oil	9127012	30322	41
Caelo	Coriander oil	10293303	30329	40
Caelo	Coriander oil	16140410	33253	40

- 63 473 spectra from a total of 1474 batches from further 439 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.

- 38 spectra from 16 *Apo-Ident* customers from 27 batches from the substance/substance group *Coriander oil*.

Supplier	Substance	Batch	Spectra
Caelo	Coriander oil	12061413	1
Caelo	Coriander oil	12228503	2
Caelo	Coriander oil	14319902	1
Caelo	Coriander oil	13288112	2
Caelo	Coriander oil	15229601	2

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Supplier	Substance	Batch	Spectra
Caelo	Coriander oil	12228509	1
Caelo	Coriander oil	152229601	1
Taoasis	Coriander oil	104709-125892	1
Caelo	Coriander oil	13288109	1
Caelo	Coriander oil	15229607	2
Caelo	Coriander oil	2081306	1
Caelo	Coriander oil	10293307	2
Caelo	Coriander oil	7021303	1
Caelo	Coriander oil	11324003	1
Caelo	Coriander oil	11324002	1
Caelo	Coriander oil	11324004	1
Caelo	Coriander oil	11324005	4
Noweda	Coriander oil	11324005	1
Caelo	Coriander oil	12228501	1
AHD, 19.07.2013	Coriander oil	12228507	1
AHD, 26.09.2013	Coriander oil	12228509	2
Taoasis	Coriander oil	32040-108625	1
Caelo	Coriander oil	18061201	1
Caelo	Coriander oil	31081203	1
Caelo	Coriander oil	14011403	1
Kaders	Coriander oil	131528	1
AHD, 05.11.2013	Coriander oil	12228510	1
Taoasis	Coriander oil	31920-1111173	1
Taoasis	Coriander oil	33485-112618	1

- 58 403 spectra from 332 *Apo-Ident* customers from a total of 20 065 batches from a further 328 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 *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 *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	80	0	34 264
Type B	0	104	17	63 473
Type C	0	33	5	58 403

The substance/substance group *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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9710 %)	85.9504 % (> 83.4711 %)
Type C	100.0000 % (> 99.5965 %)	86.8421 % (> 78.9474 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31192	31192	0.00	71.99
31407	31192	10.24	64.75

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Cypress oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31837-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cypress oil; Oleum cupressi

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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
Caelo	Cypress oil	13349109	31837	40	1606484
Caelo	Cypress oil	16130501	32183	40	9464

Validation samples

A total of 156 379 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 *Cypress oil*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 32 spectra of 2 reference samples from the substance/substance group *Cypress oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cypress oil	13349109	31837 [†]	20
Caelo	Cypress oil	16130505	not required	12

- 63 562 spectra from a total of 1475 batches from further 439 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 *Cypress oil*.
- 58 441 spectra from 332 *Apo-Ident* customers from a total of 20 092 batches from a further 329 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](#).

[†]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*.

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	80	0	34 264
Type B	0	32	0	63 562
Type C	0	0	0	58 441

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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 81.2500 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31837	31837	0.00	17.06
32183	32183	0.00	26.00

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	D-alpha tocopherol
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30485-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

D-alpha tocopherol; alpha-Tocopherolum

Special notes

When selecting the *D-alpha tocopherol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *D-alpha tocopherol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	D-alpha tocopherol	13248808	31501	39	1507770
Caelo	D-alpha tocopherol	16005002	32072	40	20160203
Fagron	D-alpha tocopherol	16D14-B05-324514	32725	40	20160422

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 119 spectra of 3 reference samples from the substance/substance group D-*alpha* tocopherol. These samples are listed above in the [calibration samples](#) section.
- 34 225 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 3 reference samples from the substance/substance group D-*alpha* tocopherol.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	D-alpha tocopherol	11313309	30485	40
Caelo	D-alpha tocopherol	13248808	31501 [†]	20
Caelo	D-alpha tocopherol	16005002	32072 [†]	20

- 63 514 spectra from a total of 1474 batches from further 439 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 23 *Apo-Ident* customers from 24 batches from the substance/substance group D-*alpha* tocopherol.

Supplier	Substance	Batch	Spectra
Caelo	D-alpha tocopherol	16005002	4
Caelo	D-alpha tocopherol	16187604	3

continued on the next page

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

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Supplier	Substance	Batch	Spectra
Caelo	D-alpha tocopherol	8705007	1
Caelo	D-alpha tocopherol	11313308	3
Caelo	D-alpha tocopherol	712015	1
Caelo	D-alpha tocopherol	11313311	2
Caelo	D-alpha tocopherol	13248803	1
Sanacorp	D-alpha tocopherol	13248801	1
Caelo	D-alpha tocopherol	14159305	1
Caelo	D-alpha tocopherol	15102606	1
Caelo	D-alpha tocopherol	15102611	1
Audor Pharma	D-alpha tocopherol	16D14-B05-322951	1
Caelo	D-alpha tocopherol	12106907	2
Caelo	D-alpha tocopherol	12106901	1
Caelo	D-alpha tocopherol	12106910	3
Caelo	D-alpha tocopherol	13248802	2
Caelo	D-alpha tocopherol	12106908	1
Caelo	D-alpha tocopherol	5012I-03257	1
Caelo	D-alpha tocopherol	11313302	1
Caelo	D-alpha tocopherol	13248801	1
Caelo	D-alpha tocopherol	132488003	1
Caelo	D-alpha tocopherol	11313301	1
Caelo	D-alpha tocopherol	14159303	1
Caelo	D-alpha tocopherol		1
Caelo	D-alpha tocopherol	11313309	1

- 58 404 spectra from 332 *Apo-Ident* customers from a total of 20 069 batches from a further 328 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 *D-alpha tocopherol* 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 *D-alpha tocopherol* 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	119	0	34 225
Type B	0	80	0	63 514
Type C	0	36	1	58 404

The substance/substance group *D-alpha tocopherol* 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 % (> 99.9691 %)	100.0000 % (> 94.9580 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5965 %)	97.2973 % (> 89.1892 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31501	31501	0.00	54.58
32072	31501	7.00	55.89
32725	31501	17.82	69.86

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Dexpanthenol**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30884-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Dexpanthenol; Dexpanthenolum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Dexpanthenol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dexpanthenol	12018707	30884	40	20120207
Caelo	Dexpanthenol	14051903	31317	40	20140319
Euro OTC	Dexpanthenol	1309030-03	31532	40	AR-15-FG-005869-01
Euro OTC	Dexpanthenol	1510008	31769	40	20151102*

Validation samples

A total of 156 379 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 *Dexpanthenol*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 157 spectra of 5 reference samples from the substance/substance group *Dexpanthenol*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Dexpanthenol	1309030-03	31532 [†]	20
Euro OTC	Dexpanthenol	1510008	31769 [†]	17
Euro OTC	Dexpanthenol	1606015	32465	40
Euro OTC	Dexpanthenol	1607027	32467	40
Euro OTC	Dexpanthenol	1610041	32829	40

- 63 437 spectra from a total of 1472 batches from further 439 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.

- 838 spectra from 208 *Apo-Ident* customers from 274 batches from the substance/substance group *Dexpanthenol*.

*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.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Dexpanthenol	1302009	1
Caelo	Dexpanthenol	1304023	1
Caelo	Dexpanthenol	4031502	1
Euro OTC	Dexpanthenol	2081403	1
Euro OTC	Dexpanthenol	4091514	1
Euro OTC	Dexpanthenol	5051504	1
Euro OTC	Dexpanthenol	7011503	1
Euro OTC	Dexpanthenol	5051505	1
Euro OTC	Dexpanthenol	10061508	1
Euro OTC	Dexpanthenol	11021503	1
Euro OTC	Dexpanthenol	1111406	1
Caelo	Dexpanthenol	12031602	1
Caelo	Dexpanthenol	12285214	6
Fagron	Dexpanthenol	13/04-N04	2
Fagron	Dexpanthenol	13/29-B05-287528	1
Fagron	Dexpanthenol	12E11-N02	19
Euro OTC	Dexpanthenol	130100902	2
Fagron	Dexpanthenol	12J30-B03-287502	1
Euro OTC	Dexpanthenol	1301009-02	7
Alliance health	Dexpanthenol	1204010-01	1
Caelo	Dexpanthenol	13084703	7
Euro OTC	Dexpanthenol	130903001	2
Euro OTC	Dexpanthenol	1309030-01	2
Caelo	Dexpanthenol	13084709	6
Caelo	Dexpanthenol	13084705	3
Caelo	Dexpanthenol	1235899	1
Phönix	Dexpanthenol	1309030-01	1
Euro OTC	Dexpanthenol	1309030-02	7
BASF AG	Dexpanthenol	1309030-01	1
Euro OTC	Dexpanthenol	130903002	1
Raben-Apotheke Mildenau	Dexpanthenol	1309030-03	1
Euro OTC	Dexpanthenol	1309030-03	1
Alliance Health 03.12.2...	Dexpanthenol	1309030-03	1
Caelo	Dexpanthenol	13189503	11
Caelo	Dexpanthenol	13342601	3
Caelo	Dexpanthenol	13342603	4
Caelo	Dexpanthenol	13189506	7
Caelo	Dexpanthenol	13342604	1
Caelo	Dexpanthenol	13342602	4
Caelo	Dexpanthenol	13342605	6
Bombastus	Dexpanthenol	13342605	1
Noweda	Dexpanthenol	13342605	1
Caelo	Dexpanthenol	13342606	11
Noweda	Dexpanthenol	13342606	1
GEHE 17.06.2014	Dexpanthenol	13342610	1
Caelo	Dexpanthenol	13342608	1
Caelo	Dexpanthenol	13342610	3
Caelo	Dexpanthenol	13342611	4
Fagron	Dexpanthenol	13D22-N12	13
Fagron	Dexpanthenol	13I04-N04	7
Fagron	Dexpanthenol	13J29-B05	8
Fagron	Dexpanthenol	13J29-B05-287526	6
Fagron	Dexpanthenol	13J29-b05-287526	1
Fagron	Dexpanthenol	13J29B05287526	1
Caelo	Dexpanthenol	13J29-B05-287526	1
Fagron	Dexpanthenol	13L02-B04	3
Fagron	Dexpanthenol	13L02-B04-292067	2
Fagron	Dexpanthenol	13J29-B05-287527	1
Fagron	Dexpanthenol	13J29-B05-287528	1
Fagron	Dexpanthenol	13L02-B04-292068	7

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Supplier	Substance	Batch	Spectra
Caelo	Dexpanthenol	14031410	1
Caelo	Dexpanthenol	14051901	1
Caelo	Dexpanthenol	14051903	5
Caelo	Dexpanthenol	14051904	5
Caelo	Dexpanthenol	14051905	4
Caelo	Dexpanthenol	14051913	1
Caelo	Dexpanthenol	14051908	3
Euro OTC	Dexpanthenol	1407039-01	5
Euro OTC	Dexpanthenol	140703901	3
Euro OTC	Dexpanthenol	14070390	1
Caelo	Dexpanthenol	1407039-01	2
BASF	Dexpanthenol	1407039-01	1
Euro OTC	Dexpanthenol	1407039-02	6
Euro OTC	Dexpanthenol	140703902	1
Alliance Health 27.03.2...	Dexpanthenol	1407039-02	1
EuRho/Noweda	Dexpanthenol	1407039-02	1
Sanacorp	Dexpanthenol	1407039-02	1
Euro OTC	Dexpanthenol	14070399-01	1
Euro OTC	Dexpanthenol	1407039-1	1
Euro OTC	Dexpanthenol	140739	1
Caelo	Dexpanthenol	14214502	2
Caelo	Dexpanthenol	14214501	2
Caelo	Dexpanthenol	142141508	1
Caelo	Dexpanthenol	14214504	6
Caelo	Dexpanthenol	14214505	6
Caelo	Dexpanthenol	14214507	3
Caelo	Dexpanthenol	14214510	3
Caelo	Dexpanthenol	14214508	2
Fagron	Dexpanthenol	14214510	1
Caelo	Dexpanthenol	14214511	2
Caelo	Dexpanthenol	14214512	3
Phoenix goettin	Dexpanthenol	14214512	1
Caelo	Dexpanthenol	1421508	1
14356201	Dexpanthenol	14356201	2
Caelo	Dexpanthenol	14356201	6
Caelo	Dexpanthenol	14356203	1
Caelo	Dexpanthenol	14356204	3
Caelo	Dexpanthenol	14356210	2
Fagron	Dexpanthenol	14E01-B11	7
Fagron	Dexpanthenol	14E01B11293623	1
Fagron	Dexpanthenol	14e01-b11-293623	1
Fagron	Dexpanthenol	14E01-B11-293624	1
Fagron	Dexpanthenol	14E01-B11-295533	1
Fagron	Dexpanthenol	14E01-B11-295544	1
Fagron	Dexpanthenol	14E01-B11-295577	2
Fagron	Dexpanthenol	14E01-b11-295544	1
Fagron	Dexpanthenol	14E01-B11-295578	6
Fagron	Dexpanthenol	14E01-B11-300068	1
A.H.D.	Dexpanthenol	14E01-B11-300068	1
Fagron	Dexpanthenol	14E01-B11-300065	1
Fagron	Dexpanthenol	14E01-B11-300068	10
Fagron	Dexpanthenol	14H05-B02-0001	1
Fagron	Dexpanthenol	14E01-B11-300068	1
apomix/Holdermann	Dexpanthenol	14H05-B02-300066	1
Fagron	Dexpanthenol	14H05-B02	1
Fagron	Dexpanthenol	14H05-B02-300069	8
Fagron	Dexpanthenol	14H05-B02-305656	1
Euro OTC	Dexpanthenol	1502019-01	12
Euro OTC	Dexpanthenol	1502010-02	1
Caelo	Dexpanthenol	1502019-01	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Dexpanthenol	150201901	1
Gehe/Euro 30.06.15	Dexpanthenol	1502019-01	1
Phönix Gotha	Dexpanthenol	1502019-01	1
Euro OTC	Dexpanthenol	1502019-02	9
Phönix Gotha	Dexpanthenol	1502019-02	1
Euro OTC	Dexpanthenol	150201902	2
Caelo	Dexpanthenol	15097701	2
Caelo	Dexpanthenol	15097703	6
Caelo	Dexpanthenol	15097704	3
Caelo	Dexpanthenol	15097705	4
Caelo	Dexpanthenol	15097708	1
Fagron	Dexpanthenol	15097709	1
Caelo	Dexpanthenol	15097709	2
Caelo	Dexpanthenol	15097710	3
Caelo	Dexpanthenol	15097711	3
Caelo	Dexpanthenol	15097712	1
Noweda	Dexpanthenol	15097712	1
Caesar & Loretz GmbH Hi...	Dexpanthenol	15097714	2
Caelo	Dexpanthenol	15097714	11
Euro OTC	Dexpanthenol	1510008-01	14
Euro OTC	Dexpanthenol	151000801	1
Gehe/ Euro	Dexpanthenol	1510008-01	1
Euro OTC	Dexpanthenol	1510008-02	6
Phoenix	Dexpanthenol	1510008-02	1
Caelo	Dexpanthenol	15260905	5
Alliance H.	Dexpanthenol	15260905	1
Caelo	Dexpanthenol	15260906	7
Caelo	Dexpanthenol	15260907	4
Euro OTC	Dexpanthenol	15260908	1
Caelo	Dexpanthenol	15395502	2
Caelo	Dexpanthenol	15395507	2
Caelo	Dexpanthenol	15395508	2
Caolo	Dexpanthenol	15395506	1
Fagron	Dexpanthenol	15A30-B08	4
Fagron	Dexpanthenol	15A30-B08-306695	3
Fagron	Dexpanthenol	15F26-B01-314370	6
Fagron	Dexpanthenol	15F26-B01-317519	1
Fagron	Dexpanthenol	15F26-B01-319991	4
Caelo	Dexpanthenol	16043502	2
Caelo	Dexpanthenol	16043504	3
Caelo	Dexpanthenol	16043503	1
Caelo	Dexpanthenol	16043505	3
DSM Nutritional Prod./...	Dexpanthenol	16043505	1
Noweda	Dexpanthenol	16043505	1
Caelo	Dexpanthenol	16043510	4
Caelo	Dexpanthenol	16043511	1
Caelo	Dexpanthenol	16043512	5
Caelo	Dexpanthenol	16043506	1
Euro OTC	Dexpanthenol	1606015-01	3
Euro/Noweda30.01.17	Dexpanthenol	1606015-01	1
Caelo	Dexpanthenol	16164808	1
Caelo	Dexpanthenol	16164810	2
Fagron	Dexpanthenol	16D07-B04-322110	1
Fagron	Dexpanthenol	16D07-B04-323096	1
Euro OTC	Dexpanthenol	17041503	1
Caelo	Dexpanthenol	2187	1
Euro OTC	Dexpanthenol	17091401	1
Caelo	Dexpanthenol	23041401	1
Sanacorp	Dexpanthenol	2/AKD4	1
Caelo	Dexpanthenol	22011511	1

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Supplier	Substance	Batch	Spectra
BASF	Dexpanthenol	2181	1
Caelo	Dexpanthenol	23081602	1
Euro OTC	Dexpanthenol	23041402	1
Caelo	Dexpanthenol	23081603	1
Euro OTC	Dexpanthenol	23101409	1
Caelo	Dexpanthenol	26081401	1
Fagron	Dexpanthenol	2914E-01082	1
Caelo	Dexpanthenol	2614E-01082	1
Euro OTC	Dexpanthenol	27031503	1
Caelo	Dexpanthenol		3
Euro OTC	Dexpanthenol	28111404	1
Euro OTC	Dexpanthenol	28071501	1
Caelo	Dexpanthenol	26081402	1
Euro OTC	Dexpanthenol	31071501	1
Fagron	Dexpanthenol	TL01203018	3
DSM Nutritional Prod./...	Dexpanthenol	TL01212052	1
Fagron	Dexpanthenol	TL01305030	7
Caelo	Dexpanthenol	2101303	1
Caelo	Dexpanthenol	3051305	1
Fagron	Dexpanthenol	TL01312070	1
Caelo	Dexpanthenol	3101202	1
sanaEuro	Dexpanthenol	311V-01082	1
Caelo	Dexpanthenol	5061306	1
Caelo	Dexpanthenol	3121303	1
Fagron	Dexpanthenol	8572983	1
Caelo	Dexpanthenol	9081206	1
Caelo	Dexpanthenol	9312203	1
Caelo	Dexpanthenol	10067908	1
Noweda	Dexpanthenol	11010703	1
Kehr	Dexpanthenol	110032-01	1
EuRho	Dexpanthenol	1107023-01	1
Euro OTC	Dexpanthenol	1110032-01	3
EuRho	Dexpanthenol	1110032-01	1
Sanacorp/ euRho	Dexpanthenol	1103053-01	1
Caelo	Dexpanthenol	11293501	2
Caelo	Dexpanthenol	11293503	1
Gehe	Dexpanthenol	11293501	1
Caelo	Dexpanthenol	11293506	3
Caelo	Dexpanthenol	11293507	4
Fagron	Dexpanthenol	11B21-N01	1
Fagron	Dexpanthenol	11B21-N01	1
Caelo	Dexpanthenol	1193507	1
Fagron	Dexpanthenol	11H26-N03	3
Caelo	Dexpanthenol	12018703	9
Caelo	Dexpanthenol	12018702	1
Caelo	Dexpanthenol	12018706	2
Caelo	Dexpanthenol	12018707	4
Caelo	Dexpanthenol	12018713	4
Caelo	Dexpanthenol	12018715	1
Caelo	Dexpanthenol	1201873	1
Euro OTC	Dexpanthenol	1204010-01	9
Phönix Gotha	Dexpanthenol	1204010-01	1
Euro OTC	Dexpanthenol	1204010-02	11
EuRho	Dexpanthenol	1204010-02	1
Caelo	Dexpanthenol	12126702	13
Caelo	Dexpanthenol	12126704	5
Caelo	Dexpanthenol	12126705	7
Anzag	Dexpanthenol	12126705	2
Caelo	Dexpanthenol	12126707	2
Phönix	Dexpanthenol	1216707	1

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Supplier	Substance	Batch	Spectra
Großhandel	Dexpanthenol	12186705	1
Caelo	Dexpanthenol	12285201	6
Caesar&lorenz,Phoenix	Dexpanthenol	12285201	1
Caelo	Dexpanthenol	1213A-01082	1
Caelo	Dexpanthenol	12285202	6
cesar&lorenz/Phönix	Dexpanthenol	12285203	1
Caelo	Dexpanthenol	12285203	3
Gehe	Dexpanthenol	12285203	1
Phönix	Dexpanthenol	12285204	1
Caelo	Dexpanthenol	12285205	1
Caelo	Dexpanthenol	12285204	2
Noweda	Dexpanthenol	12285211	2
Caelo	Dexpanthenol	12285211	8
Caelo	Dexpanthenol	12285212	2
Fagron	Dexpanthenol	12B13-N07	3
Euro OTC	Dexpanthenol	129401002	1
Fagron	Dexpanthenol	12b13-n07	1
Noweda	Dexpanthenol	12B13-N07	1
Caelo	Dexpanthenol	122852211	1
Fagron	Dexpanthenol	12813-No7	1
Gehe	Dexpanthenol	12E11-N02	2
Fagron	Dexpanthenol	12e11-n02	1
Anzag	Dexpanthenol	12E11-N02	3
Fragron	Dexpanthenol	12E11-N02	1
fargon/Sanacorp	Dexpanthenol	12E11-N02	1
Noweda	Dexpanthenol	12E11-N02	3
Fagron	Dexpanthenol	12E11-No2	1
Fagron	Dexpanthenol	12e11-N02	1
Fagron	Dexpanthenol	12H28-N07	6
Caelo	Dexpanthenol	12E11-N02	1
Anzag	Dexpanthenol	12K27-N04	1
Fagron	Dexpanthenol	12K27-N04	5
Phoenix 30.04.2013	Dexpanthenol	12H28-N07	1
Fagron	Dexpanthenol	12L28-N02	1
Fagron	Dexpanthenol	12L28-N03	5
Caelo	Dexpanthenol	12L28-N03	1
Fagron	Dexpanthenol	12L28-N03	1
Gehe	Dexpanthenol	12L28-N03	1
Fagron	Dexpanthenol	12L28-No3	1
Euro OTC	Dexpanthenol	1301009-01	17
Euro OTC	Dexpanthenol	1301009	1
Euro OTC	Dexpanthenol	1301009-001	1
Gehe	Dexpanthenol	13/04-N04	1
Alliance	Dexpanthenol	1301009-01	1
Euro OTC	Dexpanthenol	130100901	1
Daiichi Fine Chemicals	Dexpanthenol	1301009-01	1
EuRho	Dexpanthenol	1301009-01	1
Caelo	Dexpanthenol	1301009-02	1
Phönix	Dexpanthenol	1301009-02	1
Caelo	Dexpanthenol	13021305	1
Caelo	Dexpanthenol	13084702	13
Großhandel	Dexpanthenol	13084702	1
Caelo	Dexpanthenol	13084704	5
Caelo	Dexpanthenol	13084706	5
Caelo	Dexpanthenol	13084707	2
Caelo	Dexpanthenol	13084711	1
Caelo	Dexpanthenol	13091309	1
Caesar/Noweda	Dexpanthenol	13084709	1
Großhandel	Dexpanthenol	13189502	1
Caelo	Dexpanthenol	13189502	2

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Supplier	Substance	Batch	Spectra
Großhandel	Dexpanthenol	13189503	2
Caelo	Dexpanthenol	13189504	2
Noweda	Dexpanthenol	13342601	1
Sanacorp	Dexpanthenol	13342601	1
Gehe	Dexpanthenol	13D22-N12	2
Caelo	Dexpanthenol	1513F-01082	1
Caelo	Dexpanthenol	15071304	1
Caelo	Dexpanthenol	16021307	1
Caelo	Dexpanthenol	16101305	1
Caelo	Dexpanthenol	18111306	1
Caelo	Dexpanthenol	18011303	1
Caelo	Dexpanthenol	19121204	1
Caelo	Dexpanthenol	20071205	1
Caelo	Dexpanthenol	19121205	1
Caelo	Dexpanthenol	20061203	1
Caelo	Dexpanthenol	25021405	1
Caelo	Dexpanthenol	24111201	1
Caelo	Dexpanthenol	20121301	1
Caelo	Dexpanthenol	25101203	1
Caelo	Dexpanthenol	22021304	1
Caelo	Dexpanthenol	25031305	2
Caelo	Dexpanthenol	20261012-1	1
Sanacorp	Dexpanthenol	36/AKD22	1
Euroo/Ebert	Dexpanthenol	3813E-01082	1
Caelo	Dexpanthenol	3713A-01082	1
Caesar/Noweda	Dexpanthenol	4811A-01082	1
Caelo	Dexpanthenol	25101204	1
Caelo	Dexpanthenol	82729498	1
Euro OTC	Dexpanthenol	95700556P0	2
Euro OTC	Dexpanthenol	E0EIE22902	1
Euro OTC	Dexpanthenol	E0EJD41902	1
Gehe	Dexpanthenol	TL01108059	1
Fagron	Dexpanthenol	TL01110074	6
Fagron	Dexpanthenol	TL01212052	1
Caelo	Dexpanthenol	TL01110076	1
Fagron	Dexpanthenol	T1012120252	1
Fagron	Dexpanthenol	12K27-N04	1
Anzag	Dexpanthenol	12H28-N07	1
Holdermann	Dexpanthenol	13/04-N04	1
Fagron	Dexpanthenol	12e11-no2	1
EUro/AHD	Dexpanthenol	1301009-01	2
Hedinger/AHD	Dexpanthenol	1301009-02	1
A.H.D.	Dexpanthenol	13D22-N12	1
Phönix	Dexpanthenol	13J29-B05287525	1

- 57 603 spectra from 332 *Apo-Ident* customers from a total of 19 822 batches from a further 328 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 *Dexpanthenol* 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 *Dexpanthenol* 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	34 184
Type B	0	157	0	63 437
Type C	0	824	14	57 603

The substance/substance group *Dexpanthenol* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 96.1783 %)
Type C	100.0000 % (> 99.5963 %)	98.3294 % (> 97.9714 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30884	31532	3.73	146.85
31317	31532	1.69	151.38
31532	31532	0.00	154.20
31769	31769	0.00	148.78

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Dexpanthenol concentrate 50%
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30492-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dexpanthenol concentrate 50%; Dexpanthenolum 50%; Pantothenolum 50%

Special notes

When selecting the *Dexpanthenol concentrate 50%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Dexpanthenol concentrate 50%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dexpanthenol con...	12171803	30664	40	20120724
Caelo	Dexpanthenol con...	15408002	31835	40	20151211
Caelo	Dexpanthenol con...	153314	31879	40	20151014*
Caelo	Dexpanthenol con...	162483	32579	40	20160901*

Validation samples

A total of 156379 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 *Dexpanthenol concentrate 50%*. These samples are listed above in the [calibration samples](#) section.
- 34184 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 204 spectra of 6 reference samples from the substance/substance group *Dexpanthenol concentrate 50%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dexpanthenol concentrate 50%	11358202	30408	40
Caelo	Dexpanthenol concentrate 50%	11279706	30492	40
Caelo	Dexpanthenol concentrate 50%	14116302	31461	60
Caelo	Dexpanthenol concentrate 50%	15408002	31835 [†]	20
Caelo	Dexpanthenol concentrate 50%	153314	31879 [†]	20
Caelo	Dexpanthenol concentrate 50%	16248301	not required	24

- 63390 spectra from a total of 1471 batches from further 439 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.

- 214 spectra from 69 *Apo-Ident* customers from 63 batches from the substance/substance group *Dexpanthenol concentrate 50%*.

*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.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Dexpanthenol concentrate 50%	2101404	1
Caelo	Dexpanthenol concentrate 50%	11358201	2
Caelo	Dexpanthenol concentrate 50%	12081406	1
Caelo	Dexpanthenol concentrate 50%	13382102	2
Gehe 17.06.2014	Dexpanthenol concentrate 50%	13382102	1
Caelo	Dexpanthenol concentrate 50%	14020803	3
Caelo	Dexpanthenol concentrate 50%	1402003	1
Caelo	Dexpanthenol concentrate 50%	14020804	7
Audor Pharma	Dexpanthenol concentrate 50%	14116302	2
Caelo	Dexpanthenol concentrate 50%	14116302	4
Caelo	Dexpanthenol concentrate 50%	14116301	3
Sanacorp	Dexpanthenol concentrate 50%	14116302	1
Raben-Apotheke Mildenau	Dexpanthenol concentrate 50%	14116302	1
Caelo	Dexpanthenol concentrate 50%	14198101	11
Caelo	Dexpanthenol concentrate 50%	14198103	4
Caelo	Dexpanthenol concentrate 50%	14199101	1
Caelo	Dexpanthenol concentrate 50%	14275202	1
Caelo	Dexpanthenol concentrate 50%	14275203	6
Caelo	Dexpanthenol concentrate 50%	14275204	4
Caelo	Dexpanthenol concentrate 50%	14275207	3
Caelo	Dexpanthenol concentrate 50%	14373301	1
Caelo	Dexpanthenol concentrate 50%	14373302	5
Gehe	Dexpanthenol concentrate 50%	14373302	1
Caelo	Dexpanthenol concentrate 50%	15050801	2
Caelo	Dexpanthenol concentrate 50%	15050802	4
Caelo	Dexpanthenol concentrate 50%	1508002	1
Caelo	Dexpanthenol concentrate 50%	15142901	4
Caelo	Dexpanthenol concentrate 50%	15142902	3
Caelo	Dexpanthenol concentrate 50%	15196202	2
Caelo	Dexpanthenol concentrate 50%	15196203	5
Caelo	Dexpanthenol concentrate 50%	15331404	5
Caelo	Dexpanthenol concentrate 50%	15331402	1
Rondell Apotheke	Dexpanthenol concentrate 50%	15331404	1
Caelo	Dexpanthenol concentrate 50%	15408002	8
Noweda	Dexpanthenol concentrate 50%	15408002	1
Caelo	Dexpanthenol concentrate 50%	15408003	4
Caesar&Loretz GmbH	Dexpanthenol concentrate 50%	15408003	1
Bombastus	Dexpanthenol concentrate 50%	16025303	1
Caelo	Dexpanthenol concentrate 50%	1602503	1
Caelo	Dexpanthenol concentrate 50%	16025303	3
Ebert & Jacobi 01.06...	Dexpanthenol concentrate 50%	16025303	1
Caelo	Dexpanthenol concentrate 50%	16136503	7
Caelo	Dexpanthenol concentrate 50%	16136504	5
Caelo	Dexpanthenol concentrate 50%	16136505	2
Caelo	Dexpanthenol concentrate 50%	16248301	3
Caelo	Dexpanthenol concentrate 50%	16248303	1
Audor Pharma	Dexpanthenol concentrate 50%	AP65524488Q0P	2
Lamotte	Dexpanthenol concentrate 50%	AP83943088Q0P	1
Audor Pharma	Dexpanthenol concentrate 50%	AP36716516K0P	1
Audor Pharma	Dexpanthenol concentrate 50%	AP83943088Q0P	1
Caelo	Dexpanthenol concentrate 50%	11279703	1
Caelo	Dexpanthenol concentrate 50%		1
Caelo	Dexpanthenol concentrate 50%	11279704	1
Caelo	Dexpanthenol concentrate 50%	12030801	2
Gehe	Dexpanthenol concentrate 50%	11358204	1
Caelo	Dexpanthenol concentrate 50%	11358202	1
Caelo	Dexpanthenol concentrate 50%	12127003	4
Caelo	Dexpanthenol concentrate 50%	12171802	3
Caelo	Dexpanthenol concentrate 50%	12171803	5
Noweda	Dexpanthenol concentrate 50%	12171802	1

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Supplier	Substance	Batch	Spectra
Caelo	Dexpanthenol concentrate 50%	12256001	2
Caelo	Dexpanthenol concentrate 50%	12340302	2
Alliance Healthcare	Dexpanthenol concentrate 50%	12256001	1
Caelo	Dexpanthenol concentrate 50%	12256002	3
Gehe	Dexpanthenol concentrate 50%	13019203	1
Caelo	Dexpanthenol concentrate 50%	13019203	8
Noweda	Dexpanthenol concentrate 50%	12340302	1
Noweda	Dexpanthenol concentrate 50%	12340303	2
Caelo	Dexpanthenol concentrate 50%	13174702	7
Gehe	Dexpanthenol concentrate 50%	13019204	1
Caelo	Dexpanthenol concentrate 50%	13068004	3
Caelo	Dexpanthenol concentrate 50%	13068003	2
Alliance Health	Dexpanthenol concentrate 50%	13068003	1
Caelo	Dexpanthenol concentrate 50%	13019204	1
gehe 31.01.2014	Dexpanthenol concentrate 50%	13068004	1
Caelo	Dexpanthenol concentrate 50%	13174703	5
Alliance Healthcare	Dexpanthenol concentrate 50%	13174703	1
Caelo	Dexpanthenol concentrate 50%	13305003	5
Sonnenberg-Apotheke	Dexpanthenol concentrate 50%	13305004	1
Caelo	Dexpanthenol concentrate 50%	13305004	4
Audor Pharma	Dexpanthenol concentrate 50%	AP83943088QOP	1
Sanacorp	Dexpanthenol concentrate 50%	AKD29	1
Caesar&loretz,Phoenix	Dexpanthenol concentrate 50%	14116302	2
Caelo	Dexpanthenol concentrate 50%	D-050413-2	1

- 58 227 spectra from 332 *Apo-Ident* customers from a total of 20 030 batches from a further 328 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 *Dexpanthenol concentrate 50%* 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 *Dexpanthenol concentrate 50%* 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	34 184
Type B	0	204	0	63 390
Type C	0	213	1	58 227

The substance/substance group *Dexpanthenol concentrate 50%* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 97.0588 %)
Type C	100.0000 % (> 99.5963 %)	99.5327 % (> 98.1308 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30664	31879	23.32	48.78
31835	32579	3.09	57.00
31879	31879	0.00	60.95
32579	32579	0.00	58.25

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Dextrorotary lactic acid 20%
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30740-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dextrorotary lactic acid 20%; Acidum L (+)-lacticum 20%

Special notes

When selecting the *Dextrorotary lactic acid 20%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Dextrorotary lactic acid 20%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dextrorotary lac...	12105501	30740	40	1405101
Caelo	Dextrorotary lac...	15113303	31720	40	20150622

Validation samples

A total of 156 379 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 *Dextrorotary lactic acid 20%*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Dextrorotary lactic acid 20%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dextrorotary lactic acid 20%	15113303	31720 [†]	20
Caelo	Dextrorotary lactic acid 20%	161639	32341	40

- 63 534 spectra from a total of 1475 batches from further 439 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 *Dextrorotary lactic acid 20%*.

Supplier	Substance	Batch	Spectra
Caelo	Dextrorotary lactic acid 20%	15113303	1

[†]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*.

- 58 440 spectra from 332 *Apo-Ident* customers from a total of 20 091 batches from a further 328 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 *Dextrorotary lactic acid 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 *Dextrorotary lactic acid 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	80	0	34 264
Type B	0	51	9	63 534
Type C	0	1	0	58 440

The substance/substance group *Dextrorotary lactic acid 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	85.0000 % (> 80.0000 %)
Type C	100.0000 % (> 99.6053 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30740	30740	0.00	23.36
31720	30740	4.03	21.57

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Diethyl ether**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31651-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Diethyl ether

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Diethyl ether*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Hedinger	Diethyl ether	052159	31854	40	9337
Otto Fischar	Diethyl ether	5975088	31855	40	20150817

Validation samples

A total of 156 379 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 *Diethyl ether*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 4 reference samples from the substance/substance group *Diethyl ether*.

Supplier	Substance	Batch	Sample ID	Spectra
Otto Fischar	Diethyl ether	pending	30178	40
Otto Fischar	Diethyl ether	pending	30681	40
Hedinger	Diethyl ether	52159	31854 [†]	20
Otto Fischar	Diethyl ether	5975088	31855 [†]	20

- 63 474 spectra from a total of 1475 batches from further 439 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.

- 95 spectra from 57 *Apo-Ident* customers from 59 batches from the substance/substance group *Diethyl ether*.

Supplier	Substance	Batch	Spectra
Fischar	Diethyl ether	5971081	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
Hedinger	Diethyl ether	52152	1
Fischar/Gehe	Diethyl ether	5973018	1
Otto Fischar/GEHE	Diethyl ether	597301B/311152/2	1
Fischar/Gehe	Diethyl ether	597405A	1
Hedinger/Gehe	Diethyl ether	52156	2
Hedinger/ Noweda	Diethyl ether	52156	2
Hedinger	Diethyl ether	52156	1
Hedinger/Gehe	Diethyl ether	52157	1
Hedinger	Diethyl ether	14070804	1
Hedinger/Noweda	Diethyl ether	52157	3
Hedinger/Kehr	Diethyl ether	52157	1
VWR	Diethyl ether	14B110030	1
Alliance Healthcare/Fis...	Diethyl ether	5973065	1
Fischar/Noweda	Diethyl ether	5973019	1
Otto Fischar/Sanacorp	Diethyl ether	597301A	1
Fischar	Diethyl ether	5974051	1
Fischar /Zentrum-Apotheke	Diethyl ether	5974013	1
FISCHER GMBH / GEHE	Diethyl ether	5974051	1
otto fischar/Sana	Diethyl ether	597401B	1
Fischar/Phoenix	Diethyl ether	5974058	1
Stumpf/Fischer	Diethyl ether	5974052	1
noveda/fischar	Diethyl ether	5974056	1
Fischar	Diethyl ether	5974059	2
Caelo	Diethyl ether	5974058	1
Fischar	Diethyl ether	5974053	1
fischar	Diethyl ether	5975012	1
E+J, 28.09.2016	Diethyl ether	597601C	1
Otto Fischar / Sanacorp	Diethyl ether	5975015	1
Fischer/AEP	Diethyl ether	5976061	1
Otto Fischer/ Kehr	Diethyl ether	5976062	1
Phönix	Diethyl ether	52153	1
hedinger/anzag	Diethyl ether	52153	2
Hedinger	Diethyl ether	52153	4
Sanacorp	Diethyl ether	52152	1
Hebinger	Diethyl ether	52153	2
Hedinger/V.d.L.	Diethyl ether	52153	1
gepepharm GmbH	Diethyl ether	52155	1
Hedinger/Noweda	Diethyl ether	52153	1
Caelo	Diethyl ether	52156	1
Hedinger/Kehr	Diethyl ether	52156	1
Hedinger	Diethyl ether	52155	1
Fischar	Diethyl ether	52157	1
Caelo	Diethyl ether	28051304	1
Hedinger/Sanacorp	Diethyl ether	12114902	1
Noweda	Diethyl ether	5971381	1
Fischar/Sanacorp	Diethyl ether	5972042	1
Hedinger	Diethyl ether	30011406	1
Otto Fischar GmbH	Diethyl ether	5972045	1
Fischer Saarbrücken/GEHE	Diethyl ether	5972047	1
Otto Fischar GmbH	Diethyl ether	5972048	1
Phönix	Diethyl ether	597204B	1
Otto Fischar GmbH& Co.KG	Diethyl ether	5972049	1
Otto Fischar GmbH& Co.KG	Diethyl ether	597204C	1
Fischar	Diethyl ether	5972082	1
Otto Fischar GmbH	Diethyl ether	597208	1
Otto Fischar GmbH	Diethyl ether	5972082	1
Gehe	Diethyl ether	5972082	1
Otto Fischar GmbH	Diethyl ether	5972088	1
fischar	Diethyl ether	5972083	1
Fischar	Diethyl ether	5972089	1

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Supplier	Substance	Batch	Spectra
Otto Fischar Gmbh	Diethyl ether	5972089	1
Gehe/Fischar	Diethyl ether	597301	2
Fischar	Diethyl ether	597208C	1
Caelo	Diethyl ether	5973014	1
Fischar/ Now	Diethyl ether	597301C	1
Otto Fischar GmbH	Diethyl ether	597301B	1
Fischar	Diethyl ether	5973013	1
Fischar/Sanacorp	Diethyl ether	5973066	1
Fischar/Phönix	Diethyl ether	5973064	1
Phönix/Fischar	Diethyl ether	5973014	1
Fischar	Diethyl ether	5973063	1
Fischar/Anzag	Diethyl ether	5973063	1
Fischer	Diethyl ether	5973066	1
Fischar	Diethyl ether	5973069	1
Fischar	Diethyl ether	5973067	1
Phoenix/Fischarl	Diethyl ether	5973066	1
Fischar/ Now	Diethyl ether	597306C	1
Fischar	Diethyl ether	5974013	1
Fischar/Phoenix	Diethyl ether	5974014	1
Fischer	Diethyl ether	597306A	1
fischar	Diethyl ether	597601C	1
Otto Fischar	Diethyl ether	5975089	1
Fischar	Diethyl ether	597401C	1

- 58 346 spectra from 332 *Apo-Ident* customers from a total of 20 033 batches from a further 328 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 *Diethyl ether* 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 *Diethyl ether* 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	34 264
Type B	0	110	10	63 474
Type C	0	83	12	58 346

The substance/substance group *Diethyl ether* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9710 %)	91.6667 % (> 89.1667 %)
Type C	100.0000 % (> 99.5964 %)	87.3684 % (> 84.2105 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31854	31854	0.00	150.34
31855	31854	0.79	150.44

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Dimethyl isosorbide
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31750-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dimethyl isosorbide

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Dimethyl isosorbide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dimethyl isosorb...	15230402	31750	40	1603485
Caelo	Dimethyl isosorb...	15427602	31859	40	20160210

Validation samples

A total of 156 379 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 *Dimethyl isosorbide*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 92 spectra of 4 reference samples from the substance/substance group *Dimethyl isosorbide*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dimethyl isosorbide	15230402	31750 [†]	20
Caelo	Dimethyl isosorbide	15427602	31859 [†]	20
Caelo	Dimethyl isosorbide	16170904	33219	40
Caelo	Dimethyl isosorbide	16170902	not required	12

- 63 502 spectra from a total of 1473 batches from further 439 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 *Dimethyl isosorbide*.
- 58 441 spectra from 332 *Apo-Ident* customers from a total of 20 092 batches from a further 329 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](#),

[†]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 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 *Dimethyl isosorbide* 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 *Dimethyl isosorbide* 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	34 264
Type B	0	92	0	63 502
Type C	0	0	0	58 441

The substance/substance group *Dimethyl isosorbide* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 93.4783 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31750	31750	0.00	108.63
31859	31750	3.35	109.36

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Dimethyl sulfoxide
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31498-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dimethyl sulfoxide; Dimethylsulfoxidum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Dimethyl sulfoxide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Dimethyl sulfoxide	131000802	31498	40	AR-15-FG-002774-01
Fagron	Dimethyl sulfoxide	15A16-C01-16194	31732	40	20150130
Euro OTC	Dimethyl sulfoxide	1508018	31734	40	0000010817
Euro OTC	Dimethyl sulfoxide	1511013	31803	40	20151124*
Euro OTC	Dimethyl sulfoxide	1511028	31813	40	20151202*
Euro OTC	Dimethyl sulfoxide	1601048	31848	40	20160129*
Euro OTC	Dimethyl sulfoxide	1604010	32280	40	20160513*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Dimethyl sulfoxide*. These samples are listed above in the [calibration samples](#) section.
- 34 064 spectra from a total of 791 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 320 spectra of 11 reference samples from the substance/substance group *Dimethyl sulfoxide*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Dimethyl sulfoxide	131000802	31498 [†]	20
Fagron	Dimethyl sulfoxide	15A16-C01-16194	31732 [†]	20
Euro OTC	Dimethyl sulfoxide	1508018	31734 [†]	20
Euro OTC	Dimethyl sulfoxide	1511013	31803 [†]	20
Euro OTC	Dimethyl sulfoxide	1511028	31813 [†]	20
Euro OTC	Dimethyl sulfoxide	1601048	31848 [†]	20
Euro OTC	Dimethyl sulfoxide	1606007	32460	40
Euro OTC	Dimethyl sulfoxide	1608009	32707	40
Euro OTC	Dimethyl sulfoxide	1608029	32708	40
Euro OTC	Dimethyl sulfoxide	1609006	32713	40
Euro OTC	Dimethyl sulfoxide	1610015	32835	40

- 63 274 spectra from a total of 1466 batches from further 439 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](#).

*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.

[†]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*.

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.

- 329 spectra from 126 *Apo-Ident* customers from 78 batches from the substance/substance group *Dimethyl sulfoxide*.

Supplier	Substance	Batch	Spectra
Fagron	Dimethyl sulfoxide	11H30-N06	3
Fagron	Dimethyl sulfoxide	11K29-N03	3
Euro OTC	Dimethyl sulfoxide	130008-01	1
PHOENIX 06.03.2014	Dimethyl sulfoxide	1306010-01	1
Euro OTC	Dimethyl sulfoxide	1306010-01	31
Fagron	Dimethyl sulfoxide	1306010-02	1
Audor Pharma	Dimethyl sulfoxide	1306010-01D	1
Euro OTC	Dimethyl sulfoxide	1306010-02	20
Caelo	Dimethyl sulfoxide	1306010-02	1
Euro OTC	Dimethyl sulfoxide	1310008-01	19
Euro OTC	Dimethyl sulfoxide	13063010-01	1
phoenix 06.03.14	Dimethyl sulfoxide	1306010-02	1
Euro OTC	Dimethyl sulfoxide	131000801	1
Caelo	Dimethyl sulfoxide	1310008-01	2
phoenix 06.05.14	Dimethyl sulfoxide	1310008-01	1
Euro OTC	Dimethyl sulfoxide	1310008-02	14
Fagron	Dimethyl sulfoxide	1310008-02	1
Caelo	Dimethyl sulfoxide	1310008-02	1
EuRho/Phönix	Dimethyl sulfoxide	1310008-02	1
Euro	Dimethyl sulfoxide	140403-01	1
Chemical Corp./Sanacorp	Dimethyl sulfoxide	1310008-02	1
Phoenix 10.06.14	Dimethyl sulfoxide	131008-01	1
Euro OTC	Dimethyl sulfoxide	1404031-01	7
Caelo	Dimethyl sulfoxide	1404031-01	1
Gaylord/Sanacorp 28.08.14	Dimethyl sulfoxide	1404031-01	1
Chemical Corp.	Dimethyl sulfoxide	1404031-02	1
Euro OTC	Dimethyl sulfoxide	1404031-02	5
Phönix Gotha	Dimethyl sulfoxide	1404031-02	1
Euro OTC	Dimethyl sulfoxide	14051404	1
Euro/ Gehe	Dimethyl sulfoxide	1404031-02	1
Gaylord ChemicalCorp./ ...	Dimethyl sulfoxide	1404031-02	1
Euro OTC	Dimethyl sulfoxide	141039-02	1
Euro OTC	Dimethyl sulfoxide	1411039-01	9
Euro OTC	Dimethyl sulfoxide	1411039-02	3
	Dimethyl sulfoxide	1411039-02	1
Caelo	Dimethyl sulfoxide	1411039-02	3
Euro OTG/ AHD	Dimethyl sulfoxide	1411039-02	1
Euro OTC	Dimethyl sulfoxide	141103902	1
Euro OTC	Dimethyl sulfoxide	14H28-M01	2
Fagron	Dimethyl sulfoxide	14H28-M03	1
Fagron	Dimethyl sulfoxide	14H28-M01	1
Fagron	Dimethyl sulfoxide	14H28-M02	1
Euro OTC	Dimethyl sulfoxide	15011503	1
Euro OTC	Dimethyl sulfoxide	1505021	1
Phönix Gotha	Dimethyl sulfoxide	1505021-01	1
Euro OTC	Dimethyl sulfoxide	1505021-01	12
Euro OTC	Dimethyl sulfoxide	1508018-01	10
Gaylord Chemical Corp./...	Dimethyl sulfoxide	1508018-01	1
Caelo	Dimethyl sulfoxide	1508018-01	1
Euro OTC	Dimethyl sulfoxide	1508018-02	9
Euro OTC	Dimethyl sulfoxide	150801801	1
Caelo	Dimethyl sulfoxide	1508018-02	1

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Supplier	Substance	Batch	Spectra
Gaylord Chemical Corp./...	Dimethyl sulfoxide	1508018-02	1
Euro OTC	Dimethyl sulfoxide	151102801	2
AHD	Dimethyl sulfoxide	151102801	1
Euro OTC	Dimethyl sulfoxide	1511028-01	1
Phönix	Dimethyl sulfoxide	1511028-01	1
Fagron	Dimethyl sulfoxide	15A16-C01-16194	2
Euro OTC	Dimethyl sulfoxide	1601048-01	4
vitalundfitmit100/ Sana...	Dimethyl sulfoxide		1
Euro OTC	Dimethyl sulfoxide	1601048-02	2
Euro OTC	Dimethyl sulfoxide	1604010-01	5
Fagron	Dimethyl sulfoxide	15A16-C01-16195	1
Phoenix	Dimethyl sulfoxide	1601048-01	1
Bombastus	Dimethyl sulfoxide	1601048-02	1
Ebert 09.08.16 KKH	Dimethyl sulfoxide	1604010-01	1
Ebert 12.08.16	Dimethyl sulfoxide	1604040-01	1
Euro OTC	Dimethyl sulfoxide	1606007-01	2
Sanacorp	Dimethyl sulfoxide	160600701	1
Ebert KKH29.09.16	Dimethyl sulfoxide	16060074-01	1
Audor Pharma	Dimethyl sulfoxide	AP1306010-01D	3
Euro OTC	Dimethyl sulfoxide	1609006-01	1
Euro OTC	Dimethyl sulfoxide	1813A-01336	1
Euro OTC	Dimethyl sulfoxide	2071301	1
Euro OTC	Dimethyl sulfoxide	2071302	1
Euro OTC	Dimethyl sulfoxide	SYN140623	1
Euro OTC	Dimethyl sulfoxide	613A-01336	1
Euro OTC	Dimethyl sulfoxide	5111303	1
Euro OTC	Dimethyl sulfoxide	1106006-01	4
Alliance Health 06.09.2...	Dimethyl sulfoxide	10G26-N12	1
Euro OTC	Dimethyl sulfoxide	110600601	1
Euro OTC	Dimethyl sulfoxide	1004041-01	1
ANZAG am 21.05.2012	Dimethyl sulfoxide	1111059-01	2
Noweda	Dimethyl sulfoxide	1111059-01	1
Euro OTC	Dimethyl sulfoxide	1111059-01	1
Gehe	Dimethyl sulfoxide	1111059-01	1
Phönix Gotha	Dimethyl sulfoxide	1111059-02	1
EuRho	Dimethyl sulfoxide	1111059-02	1
Euro OTC	Dimethyl sulfoxide	1111059-02	1
Noweda	Dimethyl sulfoxide	1111059-02	1
Fagron	Dimethyl sulfoxide	11A21-N03	1
Gehe	Dimethyl sulfoxide	1111059-02	1
Fagron	Dimethyl sulfoxide	11E03-M04	2
Fagron	Dimethyl sulfoxide	11G18-N15	1
Euro OTC	Dimethyl sulfoxide	1207008-01	2
Euro OTC	Dimethyl sulfoxide	1207008-02	7
Sanacorp	Dimethyl sulfoxide	1207008-01	1
Euro OTC	Dimethyl sulfoxide	1210059-01	21
Großhandel	Dimethyl sulfoxide	1210059-01	1
EuRho	Dimethyl sulfoxide	1210059-01	1
Alliance Healthcare	Dimethyl sulfoxide	1210059-01	1
gaylord	Dimethyl sulfoxide	1210059-01	1
Euro OTC	Dimethyl sulfoxide	121005901	1
Gehe 18.06.2013	Dimethyl sulfoxide	1210059-01	1
Phönix	Dimethyl sulfoxide	1210059-01	1
Phoenix 23.08.2012	Dimethyl sulfoxide	12a09-N03	1
Euro OTC	Dimethyl sulfoxide	12101202	1
Euro OTC	Dimethyl sulfoxide	1303010-01	15
Euro OTC	Dimethyl sulfoxide	13003010-01	1
Euro OTC	Dimethyl sulfoxide	13011403	1
Caelo	Dimethyl sulfoxide	1306010-01	1
Gaylord/Sanacorp	Dimethyl sulfoxide	1306010-01	1

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Supplier	Substance	Batch	Spectra
Alliance Health 04.11.2...	Dimethyl sulfoxide	1306010-01	1
Euro/ Fiebig	Dimethyl sulfoxide	1306010-02	1
AHD,17.10.13	Dimethyl sulfoxide	1306010-02	1
gehe 07.01.2014	Dimethyl sulfoxide	1306010-02	2
Phönix	Dimethyl sulfoxide	1310008-01	1
Fagron	Dimethyl sulfoxide	13071201	1
Caelo	Dimethyl sulfoxide	131000801	1
Euro OTC	Dimethyl sulfoxide	1404031	1
Caelo	Dimethyl sulfoxide	29081202	1
Audor Pharma	Dimethyl sulfoxide	AP1303010-01D	1
Fagron	Dimethyl sulfoxide	27061203	1
Phönix	Dimethyl sulfoxide	AP1303010-01D	1
Fagron	Dimethyl sulfoxide	PHS1000510	1
Audor Pharma	Dimethyl sulfoxide	ap130301001d	1
Euro OTC	Dimethyl sulfoxide	26011301	1
Euro OTC	Dimethyl sulfoxide	PHS111205	1
Euro OTC	Dimethyl sulfoxide		1
Sanacorp/ PZN08597061	Dimethyl sulfoxide	1306010-01-339413100	1
Sanacorp	Dimethyl sulfoxide	1306010-02	1
Audor Pharma	Dimethyl sulfoxide	AP1210059-01D	1
Phönix/EuRho	Dimethyl sulfoxide	1207008-01	1

- 58 112 spectra from 332 *Apo-Ident* customers from a total of 20 014 batches from a further 328 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 *Dimethyl sulfoxide* 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 *Dimethyl sulfoxide* 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	34 064
Type B	0	320	0	63 274
Type C	0	307	22	58 112

The substance/substance group *Dimethyl sulfoxide* 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 % (> 99.9689 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.5963 %)	93.3131 % (> 92.4012 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31498	31498	0.00	147.12
31732	31848	1.65	151.07
31734	31734	0.00	151.13
31803	31803	0.00	152.20
31813	31813	0.00	152.14
31848	31848	0.00	151.11
32280	32280	0.00	156.45

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Dimeticon 100 / 350 / 1000**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30660-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Dimeticon 100 / 350 / 1000; Dimeticone 100; Dimeticone 1000; Dimeticone 350; Dimeticonum 100; Dimeticonum 1000; Dimeticonum 350

Special notes

When selecting the *Dimeticon 100 / 350 / 1000* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Dimeticon 100 / 350 / 1000*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dimeticone 100	12140101	30660	40	1403158
Caelo	Dimeticone 100	13049608	31333	40	20130301
Caelo	Dimeticone 350	13236306	31334	40	AR-15-FG-009277-01
Fagron	Dimeticone 350	14C20-B05-292285	31659	40	20140331
Caelo	Dimeticone 1000	161307	32169	40	20160427*
Caelo	Dimeticone 1000	15349907	32587	40	20151106
Euro OTC	Dimeticone 350	1702002	33234	40	20170302*

Validation samples

A total of 156379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Dimeticon 100 / 350 / 1000*. These samples are listed above in the [calibration samples](#) section.
- 34064 spectra from a total of 791 batches from further 222 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 200 spectra of 6 reference samples from the substance/substance group *Dimeticon 100 / 350 / 1000*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dimeticone 350	10111314	30245	40
Fagron	Dimeticone 350	14C20-B05-292285	31659 [†]	20
Caelo	Dimeticone 1000	161307	32169 [†]	20
Caelo	Dimeticone 350	160754	32208	40
Caelo	Dimeticone 100	15199409	32304	40
Fagron	Dimeticone 1000	14C20-B04-306781	32485	40

- 63394 spectra from a total of 1471 batches from further 437 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.

*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.

[†]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*.

- 92 spectra from 40 *Apo-Ident* customers from 41 batches from the substance/substance group *Dimeticone 100 / 350 / 1000*.

Supplier	Substance	Batch	Spectra
Caelo	Dimeticone 350	13049802	2
Caelo	Dimeticone 350	13236302	2
Caelo	Dimeticone 350	13236306	13
Euro OTC	Dimeticone 350	1407004-01	1
Caelo	Dimeticone 350	14074509	13
Caelo	Dimeticone 350	14074512	9
Jenne	Dimeticone 350	14074509	1
Caelo	Dimeticone 350	14074518	1
Caelo	Dimeticone 350	14336402	2
Fagron	Dimeticone 350	14C20-B05-292285	3
Ph.Eur.8.0	Dimeticone 350	14C20B05292285	1
EuRo/Phönix	Dimeticone 350	1207015-01	1
Caelo	Dimeticone 350	14704509	1
Caelo	Dimeticone 350	13236308	2
Caelo	Dimeticone 350	14336403	1
Euro OTC	Dimeticone 350	14C20-B05-292285	1
Caelo	Dimeticone 350	13049803	2
Fargon	Dimeticone 350	14C20-B05292282	1
Caelo	Dimeticone 350	13049813	1
Caelo	Dimeticone 350	13236312	2
Gehe	Dimeticone 350	1407004-01	1
Caelo	Dimeticone 350	14074511	1
Caelo	Dimeticone 100	12310801	1
Caelo	Dimeticone 100	12140101	1
Caelo	Dimeticone 100	11215905	1
Fagron	Dimeticone 350	14C20-B05	1
Noweda	Dimeticone 100	12316701	1
Fagron	Dimeticone 350	9B10	1
Caelo	Dimeticone 350	9371810	1
Caelo	Dimeticone 350	10111314	1
Caelo	Dimeticone 350	11042104	2
Caelo	Dimeticone 350	12186301	1
Euro OTC	Dimeticone 350	1207015-02	1
Euro OTC	Dimeticone 350	1207015-01	1
Anzag 24.01.2013	Dimeticone 350	12186301	1
Großhandel	Dimeticone 350	11317804	1
Kehr	Dimeticone 350	1207015-01	1
Caelo	Dimeticone 350	12193302	1
Caelo	Dimeticone 350	12193303	2
Caelo	Dimeticone 350	12193307	2
Caelo	Dimeticone 350	12193308	1
Caelo	Dimeticone 350	12193313	1
Caelo	Dimeticone 350	12193315	1
AHD, 07.11.13	Dimeticone 350	13049804	1
Caelo	Dimeticone 350	13049804	2
Caelo	Dimeticone 350	13049809	1
Fagron	Dimeticone 350	3111Q-02251	1
Caelo	Dimeticone 350		1

- 58 349 spectra from 332 *Apo-Ident* customers from a total of 20 052 batches from a further 327 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 *Dimeticon 100 / 350 / 1000* 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 *Dimeticon 100 / 350 / 1000* 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	34 064
Type B	0	192	8	63 394
Type C	0	88	4	58 349

The substance/substance group *Dimeticon 100 / 350 / 1000* 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 % (> 99.9689 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9710 %)	96.0000 % (> 94.5000 %)
Type C	100.0000 % (> 99.5964 %)	95.6522 % (> 92.3913 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30660	30660	0.00	326.79
31333	32169	1.60	327.81
31334	31334	0.00	327.93
31659	32169	2.41	325.74
32169	32169	0.00	328.61
32587	33234	2.66	325.98
33234	33234	0.00	325.04

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Ethanol 90% pure / denatured**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30379-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ethanol 90% pure / denatured; Ethanolum 90% rein / vergällt

Special notes

When selecting the *Ethanol 90% pure / denatured* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 90% pure / denatured*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
apomix	Ethanol 90% pure...	25A040913	31056	40	1404654
Caelo	Ethanol 90% pure...	14052802	31392	40	20140225
Caelo	Ethanol 90% pure...	163144	33102	40	20161209*

Validation samples

A total of 156379 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 *Ethanol 90% pure / denatured*. These samples are listed above in the [calibration samples](#) section.
- 34224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 200 spectra of 5 reference samples from the substance/substance group *Ethanol 90% pure / denatured*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ethanol 90% pure / denatured	11069005	30319	40
Caelo	Ethanol 90% pure / denatured	11329301	30379	40
Caelo	Ethanol 90% pure / denatured	161944	32324	40
Caelo	Ethanol 90% pure / denatured	163142	33103	40
Caelo	Ethanol 90% pure / denatured	163143	33104	40

- 63394 spectra from a total of 1472 batches from further 439 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.

- 289 spectra from 108 *Apo-Ident* customers from 188 batches from the substance/substance group *Ethanol 90% pure / denatured*.

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

Supplier	Substance	Batch	Spectra
Apomix	Ethanol 90% pure / denatured	2A130114	1
Caelo	Ethanol 90% pure / denatured	814E-03042	1
Anzag am 29.01.2013	Ethanol 90% pure / denatured	12068403	2
Caelo	Ethanol 90% pure / denatured	5A130214	1
Zentrum-Apotheke	Ethanol 90% pure / denatured	514I-03042	1
Caelo	Ethanol 90% pure / denatured	12355401	4
Caelo	Ethanol 90% pure / denatured	12275402	2
Anzag 28.03.2013	Ethanol 90% pure / denatured	12355601	1
Caelo	Ethanol 90% pure / denatured	12355501	2
Caelo	Ethanol 90% pure / denatured	13019601	1
Caelo	Ethanol 90% pure / denatured	12355601	4
Apotärze/Zentrum	Ethanol 90% pure / denatured	10092013-D	1
Caelo	Ethanol 90% pure / denatured	13019602	1
Caelo	Ethanol 90% pure / denatured	13019701	2
Phoenix	Ethanol 90% pure / denatured	13019703	1
Caelo	Ethanol 90% pure / denatured	13085901	3
Caelo	Ethanol 90% pure / denatured	13019703	2
Caelo	Ethanol 90% pure / denatured	1305801	1
Caelo	Ethanol 90% pure / denatured	13086001	4
Caelo	Ethanol 90% pure / denatured	13160501	2
Caelo	Ethanol 90% pure / denatured	13160601	4
Caelo	Ethanol 90% pure / denatured	13086002	1
Caelo	Ethanol 90% pure / denatured	13160701	2
Caelo	Ethanol 90% pure / denatured	13290202	2
Caelo	Ethanol 90% pure / denatured	13290201	4
Caelo	Ethanol 90% pure / denatured	13290402	3
Caesar & Loretz GmbH, 4...	Ethanol 90% pure / denatured	13290202	1
Noweda	Ethanol 90% pure / denatured	13290203	1
Caelo	Ethanol 90% pure / denatured	13290301	2
Caelo	Ethanol 90% pure / denatured	13290203	1
Caelo	Ethanol 90% pure / denatured	13160703	2
Phönix	Ethanol 90% pure / denatured	13399604	1
Caelo	Ethanol 90% pure / denatured	13399606	2
Caelo	Ethanol 90% pure / denatured	13399605	4
Phoenix	Ethanol 90% pure / denatured	13399802	1
Caelo	Ethanol 90% pure / denatured	13399801	1
Caelo	Ethanol 90% pure / denatured	14027502	1
Phonix	Ethanol 90% pure / denatured	14052601	1
Post-Apotheke 15.01.2014	Ethanol 90% pure / denatured	15012014	1
Caelo	Ethanol 90% pure / denatured	15442801	2
Gütte/Phönix	Ethanol 90% pure / denatured	20112013-M	1
Post-Apotheke	Ethanol 90% pure / denatured	1713Q-03042	1
Apomix	Ethanol 90% pure / denatured	37A101212	1
Hirsch	Ethanol 90% pure / denatured	5013Q-02303	3
Apotärze	Ethanol 90% pure / denatured	4513M-02303	1
phönix	Ethanol 90% pure / denatured		1
Caelo	Ethanol 90% pure / denatured	AKD6	1
Martinus-Apotheke	Ethanol 90% pure / denatured	A-160913-2D	2
Hustadt Apotheke	Ethanol 90% pure / denatured	Defektur	1
Martinus-Apotheke	Ethanol 90% pure / denatured	E-040414-1D	2
Martinus-Apotheke	Ethanol 90% pure / denatured	E-080114-1D	2
Mühlen-Apotheke	Ethanol 90% pure / denatured	213Q-02303	1
Caelo	Ethanol 90% pure / denatured	11329402	1
Herstellung	Ethanol 90% pure / denatured	110416P1	1
Eigenherstellung	Ethanol 90% pure / denatured	4161112	1
Caelo	Ethanol 90% pure / denatured	11329304	1
Gehe	Ethanol 90% pure / denatured	12068201	1
Caelo	Ethanol 90% pure / denatured	12068301	1
Caelo	Ethanol 90% pure / denatured	12144401	1
Caesar & Loretz GmbH, 4...	Ethanol 90% pure / denatured	12068301	1

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Supplier	Substance	Batch	Spectra
Caelo	Ethanol 90% pure / denatured	12275301	1
Caelo	Ethanol 90% pure / denatured	12355504	1
Caesar & Loretz GmbH, 4...	Ethanol 90% pure / denatured	12275402	1
Phönix Gotha	Ethanol 90% pure / denatured	20A030712	1
Phönix 27.08.2012	Ethanol 90% pure / denatured	12144402	1
Anzag 06.10.12	Ethanol 90% pure / denatured	25A290812	1
apomix	Ethanol 90% pure / denatured	22a080911	1
Fagron	Ethanol 90% pure / denatured	270614P1	1
Apomix	Ethanol 90% pure / denatured	32A141211	1
Caelo	Ethanol 90% pure / denatured	10250602	1
Caelo	Ethanol 90% pure / denatured	13085801	1
Mühlen-Apotheke	Ethanol 90% pure / denatured	4012M-02303	1
Gutenberg-Apotheke	Ethanol 90% pure / denatured	Defektur	1
Caelo	Ethanol 90% pure / denatured	12068202	1
Caelo	Ethanol 90% pure / denatured	13290401	2
Caelo	Ethanol 90% pure / denatured	14027401	3
Eigenherstellung	Ethanol 90% pure / denatured	4733	1
Caelo	Ethanol 90% pure / denatured	14208801	3
Caelo	Ethanol 90% pure / denatured	15150701	3
HirschApotheke	Ethanol 90% pure / denatured	10151-02303	1
Hirsch	Ethanol 90% pure / denatured	11233	1
Eigenherstellung	Ethanol 90% pure / denatured	115Q-07057	1
Caelo	Ethanol 90% pure / denatured	713E-02303	1
apomix	Ethanol 90% pure / denatured	7A170215	1
Apomix / Phönix	Ethanol 90% pure / denatured	5A130214	1
Eigenherstellung	Ethanol 90% pure / denatured	217I-02303	1
Caelo	Ethanol 90% pure / denatured	13399701	1
Kastner	Ethanol 90% pure / denatured	1314I-03042	1
Kastner (eigen)	Ethanol 90% pure / denatured	1215I-02303	1
Caelo	Ethanol 90% pure / denatured	13399802	1
Caelo	Ethanol 90% pure / denatured	13399803	2
Apomix / Alliance Healt...	Ethanol 90% pure / denatured	13A170516	1
Caelo	Ethanol 90% pure / denatured	14027301	1
Caelo	Ethanol 90% pure / denatured	14027303	1
Caelo	Ethanol 90% pure / denatured	14027402	1
Caelo	Ethanol 90% pure / denatured	14027501	2
GEHE 16.05.2014	Ethanol 90% pure / denatured	14027502	2
Caelo	Ethanol 90% pure / denatured	14052701	2
Caelo	Ethanol 90% pure / denatured	14052601	3
Caelo	Ethanol 90% pure / denatured	14052801	3
Caelo	Ethanol 90% pure / denatured	14052802	2
Caelo	Ethanol 90% pure / denatured	14060201	4
Caelo	Ethanol 90% pure / denatured	14060301	3
Caelo	Ethanol 90% pure / denatured	14122101	2
Caelo	Ethanol 90% pure / denatured	14122202	1
Caelo	Ethanol 90% pure / denatured	14060302	1
Caelo	Ethanol 90% pure / denatured	14122201	3
Caelo	Ethanol 90% pure / denatured	14122401	3
Caelo	Ethanol 90% pure / denatured	14122302	3
Caelo	Ethanol 90% pure / denatured	14208702	1
Caelo	Ethanol 90% pure / denatured	14208901	2
Caelo	Ethanol 90% pure / denatured	15014002	5
Caelo	Ethanol 90% pure / denatured	15010501	1
Caelo	Ethanol 90% pure / denatured	15010503	1
Caelo	Ethanol 90% pure / denatured	15014001	1
Caelo	Ethanol 90% pure / denatured	15010502	1
Caelo	Ethanol 90% pure / denatured	15010504	1
Römer-Apotheke	Ethanol 90% pure / denatured	150428003	1
Stern	Ethanol 90% pure / denatured	150622004	1
Caelo	Ethanol 90% pure / denatured	15073201	3

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Supplier	Substance	Batch	Spectra
Caelo	Ethanol 90% pure / denatured	15073202	1
Caelo	Ethanol 90% pure / denatured	15073203	1
Caelo	Ethanol 90% pure / denatured	15080301	2
Eigenherstellung	Ethanol 90% pure / denatured	1515I-02303	1
Caelo	Ethanol 90% pure / denatured	15219501	1
Libellen Apotheke	Ethanol 90% pure / denatured	1515Q-02303	1
Caelo	Ethanol 90% pure / denatured	15150704	2
Caelo	Ethanol 90% pure / denatured	15219302	1
Caelo	Ethanol 90% pure / denatured	15328201	2
Noweda	Ethanol 90% pure / denatured	15219302	1
Caelo	Ethanol 90% pure / denatured	15328301	3
Noweda	Ethanol 90% pure / denatured	15328301	1
Noweda	Ethanol 90% pure / denatured	15442602	1
Caelo	Ethanol 90% pure / denatured	15442601	2
Caelo	Ethanol 90% pure / denatured	15442602	2
Noweda	Ethanol 90% pure / denatured	15442603	1
Caelo	Ethanol 90% pure / denatured	15328401	1
Caelo	Ethanol 90% pure / denatured	15442702	1
Caelo	Ethanol 90% pure / denatured	15442703	1
Caelo	Ethanol 90% pure / denatured	16106802	1
Eigenherstellung Hubert...	Ethanol 90% pure / denatured	2014072222DF	1
apomix	Ethanol 90% pure / denatured	18A080615	1
Eigenherstellung	Ethanol 90% pure / denatured	1716Q-02303	1
Apomix/Phönix	Ethanol 90% pure / denatured	16A210610	1
Audor Pharma	Ethanol 90% pure / denatured	1614E-03042	1
Gehe	Ethanol 90% pure / denatured	16106901	1
Defektur	Ethanol 90% pure / denatured	2115A-03042	1
Caelo	Ethanol 90% pure / denatured	2515A-03042	1
Eigenherstellung	Ethanol 90% pure / denatured	2614I-02303	1
Defektur	Ethanol 90% pure / denatured	3015M-03042	1
apomix PKH GmbH Halle	Ethanol 90% pure / denatured	30A310815	1
Kastner (eigen)	Ethanol 90% pure / denatured	3114E-03042	1
Apotheke	Ethanol 90% pure / denatured	3116Q-03042	1
Eigenherstellung	Ethanol 90% pure / denatured	3416E-02303	1
Eigenherstellung	Ethanol 90% pure / denatured	3416E-07057	1
Apotärze	Ethanol 90% pure / denatured	4414E-03042	1
Eigen/Neue Apotheke	Ethanol 90% pure / denatured	4315I-02303	1
Rondell Apotheke	Ethanol 90% pure / denatured	4615E-02303	1
Engel/Engel	Ethanol 90% pure / denatured	4415A-07014	1
Eigenherstellung	Ethanol 90% pure / denatured	4414A-07057	1
Rondell Apotheke	Ethanol 90% pure / denatured	4615E-07209	1
Rondell Apotheke	Ethanol 90% pure / denatured	4615E-03042	1
Defektur	Ethanol 90% pure / denatured	4714E-03042	1
Rondell Apotheke	Ethanol 90% pure / denatured	4814E-02303	1
Caelo	Ethanol 90% pure / denatured	80933148	1
Martinus-Apotheke	Ethanol 90% pure / denatured	E-021116-3D	1
Martinus-Apotheke	Ethanol 90% pure / denatured	E-160416-1D	1
Defektur	Ethanol 90% pure / denatured	5015I-03042	1
Martinus-Apotheke	Ethanol 90% pure / denatured	E-030117-1Praxis	1
Martinus-Apothke	Ethanol 90% pure / denatured	E-170215-1D	1
Martinus-Apotheke	Ethanol 90% pure / denatured	E-130216-1D	1
Martinus-Apotheke	Ethanol 90% pure / denatured	E-211014-1D	1
Defektur	Ethanol 90% pure / denatured	60616/50Hk	1
Martinus-Apotheke	Ethanol 90% pure / denatured	E-220716-1P	1
	Ethanol 90% pure / denatured		2
	Ethanol 90% pure / denatured	Hergestellt070514	1
Eigenherstellung	Ethanol 90% pure / denatured	4211215	1
Caelo	Ethanol 90% pure / denatured	12275501	1
Fagron	Ethanol 90% pure / denatured	14027303	2
Gutenberg-Apotheke	Ethanol 90% pure / denatured	140324001	1

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Supplier	Substance	Batch	Spectra
Caelo	Ethanol 90% pure / denatured	15442502	1
Eigenherstellung	Ethanol 90% pure / denatured	1312I-07057	1
Eigenherstellung	Ethanol 90% pure / denatured	514E-07057	2
Eigenherstellung	Ethanol 90% pure / denatured	1613A-07057	1
Eigenherstellung	Ethanol 90% pure / denatured	4313Q-07057	1
Eigenherstellung	Ethanol 90% pure / denatured	4713Q-07057	2
Apomix	Ethanol 90% pure / denatured	12A150513	1
Defektur	Ethanol 90% pure / denatured	30082012	1
Defektur	Ethanol 90% pure / denatured	26112012D01	1
Caelo	Ethanol 90% pure / denatured	814E-02303	1
Caelo	Ethanol 90% pure / denatured	915Q-02303	1
Hustadt apotheke	Ethanol 90% pure / denatured	130612/1	1
Post-Apotheke	Ethanol 90% pure / denatured	1414A-02303	1
Defektur	Ethanol 90% pure / denatured	1816A-03042	1
Caelo	Ethanol 90% pure / denatured	1915L-02303	1
Defektur	Ethanol 90% pure / denatured	3216N-03042	1
Defektur	Ethanol 90% pure / denatured	4916E-03042	1
Caelo	Ethanol 90% pure / denatured	5214E-02303	1
Caelo	Ethanol 90% pure / denatured	2413Q-03042	1
Römer-Apotheke	Ethanol 90% pure / denatured	1914E-03042	1
Römer-Apotheke	Ethanol 90% pure / denatured	36141-03042	1
Germania Apo	Ethanol 90% pure / denatured	219060	1
Rondell-Apotheke	Ethanol 90% pure / denatured	3913Q-03042	1
Römer-Apotheke	Ethanol 90% pure / denatured	4213E-03042	1

- 58 152 spectra from 332 *Apo-Ident* customers from a total of 19 907 batches from a further 328 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 90% pure / denatured* 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 90% pure / denatured* 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	34 224
Type B	0	200	0	63 258
Type C	0	284	5	58 057

The substance/substance group *Ethanol 90% pure / denatured* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9714 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.5979 %)	98.2699 % (> 97.2318 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31056	31056	0.00	71.51
31392	31056	12.05	78.00
33102	33102	0.00	69.78

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Ethanol 96% pure / denatured**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31488-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ethanol 96% pure / denatured; Ethanolum 96% rein / vergällt

Special notes

When selecting the *Ethanol 96% pure / denatured* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 96% pure / denatured*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Merck KGaA	Ethanol 96% pure...	K45197671406	31488	40	1503676
Laborchemie A...	Ethanol 96% pure...	21001382	31564	40	20100725

Validation samples

A total of 156379 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 *Ethanol 96% pure / denatured*. These samples are listed above in the [calibration samples](#) section.
- 34264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 3 reference samples from the substance/substance group *Ethanol 96% pure / denatured*.

Supplier	Substance	Batch	Sample ID	Spectra
Laborchemie Apolda	Ethanol 96% pure / denatured	16000409	30534	40
Merck	Ethanol 96% pure / denatured	K45197671406	31488 [†]	20
Laborchemie Apolda	Ethanol 96% pure / denatured	21001382	31564 [†]	20

- 63514 spectra from a total of 1474 batches from further 439 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.

- 451 spectra from 142 *Apo-Ident* customers from 285 batches from the substance/substance group *Ethanol 96% pure / denatured*.

Supplier	Substance	Batch	Spectra
Alkoholvertrieb Dr. Ber...	Ethanol 96% pure / denatured	15132014/02122013	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
hetterich	Ethanol 96% pure / denatured	3574702	1
Alkoholvertrieb Süd GmbH	Ethanol 96% pure / denatured	2/0713	1
Branntweinmonopol	Ethanol 96% pure / denatured	613Et0H96	1
Applichem/Diagonal	Ethanol 96% pure / denatured	70214PJK05	1
Bundesmonopolverwaltung...	Ethanol 96% pure / denatured		10
Bombastus	Ethanol 96% pure / denatured		1
Caelo	Ethanol 96% pure / denatured	1/12	1
Bergchemie	Ethanol 96% pure / denatured		2
Bergchemie	Ethanol 96% pure / denatured	13/03/06	2
Kassner & Sasse	Ethanol 96% pure / denatured	12/11/23	1
Kottkamp/Gehe	Ethanol 96% pure / denatured	121213	1
Berkel AHK	Ethanol 96% pure / denatured	13/07/17-1	1
BfB	Ethanol 96% pure / denatured	1/2/3/4	1
Berkel AHK	Ethanol 96% pure / denatured	13/11/08	1
Alkoholvertrieb Süd GmbH...	Ethanol 96% pure / denatured	1313081029/26082013	1
kottkamp,gehe	Ethanol 96% pure / denatured	130513	1
Bergchemie	Ethanol 96% pure / denatured	14-08-12	2
BMV Branntwein	Ethanol 96% pure / denatured		12
Berkel AHK	Ethanol 96% pure / denatured	1410T31040613	1
Berkel AHK	Ethanol 96% pure / denatured	1410T311060513	1
Noweda	Ethanol 96% pure / denatured	19000663	2
Berkel AHK	Ethanol 96% pure / denatured	1410T31191113	1
Tereos 20131470D	Ethanol 96% pure / denatured	1410T31040613	1
Miller	Ethanol 96% pure / denatured	1413040904/16042013	1
Bergchemie	Ethanol 96% pure / denatured	13/11/27	1
Laborchemi Apolda	Ethanol 96% pure / denatured	19002423	1
Laborchemie Apolda	Ethanol 96% pure / denatured	20000065	1
Laborchemie/Gehe	Ethanol 96% pure / denatured	20000305	3
Apolda GmbH	Ethanol 96% pure / denatured	19001936	1
Apolda GmbH	Ethanol 96% pure / denatured	20000305	1
Heyl	Ethanol 96% pure / denatured	20000947	1
Laborchemie/Gehe	Ethanol 96% pure / denatured	20000071	1
Noweda / Apolda	Ethanol 96% pure / denatured	20000974	2
Apolda / Gehe	Ethanol 96% pure / denatured	20000974	1
Gehe/Laborchemie Apolda	Ethanol 96% pure / denatured	20000973	1
Gehe 18.04.2013	Ethanol 96% pure / denatured	20000065	1
Spangro/Laborchemie Apo...	Ethanol 96% pure / denatured	20001583	1
Laborchemie Apolda/Noweda	Ethanol 96% pure / denatured	20000974	1
Sanacorp	Ethanol 96% pure / denatured	20001574	1
Noweda/Labochemie	Ethanol 96% pure / denatured	20001566	2
Heyl / AHD	Ethanol 96% pure / denatured	20001830	1
Laborchemie APOLDA/ Now...	Ethanol 96% pure / denatured	20001574	1
Apolda, Noweda	Ethanol 96% pure / denatured	20001212	1
Laborchemie Apolda	Ethanol 96% pure / denatured	20001886	2
Laborchemie Apolda Heyl...	Ethanol 96% pure / denatured	20001887	1
Laborchemie Apolda	Ethanol 96% pure / denatured	20002191	1
Gehe am 18.02.2014	Ethanol 96% pure / denatured	20002191	1
W. Hoffmann/Noweda	Ethanol 96% pure / denatured	20120106	2
Apolda / Sanacorp	Ethanol 96% pure / denatured	20002191	1
Schmittmann GmbH	Ethanol 96% pure / denatured	20130105	1
Bundesmonopolverw.	Ethanol 96% pure / denatured	20130903	2
Caelo	Ethanol 96% pure / denatured	2310A0341	1
Werner Hofmann	Ethanol 96% pure / denatured	30091302	1
Berkel AHK	Ethanol 96% pure / denatured	3613Q2304	1
Apolda/Phönix	Ethanol 96% pure / denatured	3613M-02304	1
Kost/kost/sophien	Ethanol 96% pure / denatured	4065280513	1
kost	Ethanol 96% pure / denatured	410031212057	1
Kost/Krieger/04.07.13	Ethanol 96% pure / denatured	410040713061	2
kost	Ethanol 96% pure / denatured	410031212052	1
Kost/Krieger/07.01.14	Ethanol 96% pure / denatured	410051213065	4

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Supplier	Substance	Batch	Spectra
Sophien-Arzneimittel/dir. ...	Ethanol 96% pure / denatured	410081013063	2
Kost/kost/sophien	Ethanol 96% pure / denatured	410051213065	2
Kost/Krieger/06.12.13	Ethanol 96% pure / denatured	410111113064	3
Kost/Krieger/14.10.13	Ethanol 96% pure / denatured	410090813062	3
Kost/Krieger/12.08.13	Ethanol 96% pure / denatured	410130313059	2
Kost/Krieger/26.06.13	Ethanol 96% pure / denatured	410140513060	1
Kost/Krieger/26.06.13	Ethanol 96% pure / denatured	410150513060	1
Kost/Krieger/18.03.14	Ethanol 96% pure / denatured	410220114066	3
Brüggenmann/Alkohol	Ethanol 96% pure / denatured	7814020283	1
Brüggenmann/Alkohol	Ethanol 96% pure / denatured	7814060362	1
Sonnenberg/Zentrum	Ethanol 96% pure / denatured	4711E-03041	1
Werner Hoffmann	Ethanol 96% pure / denatured	Ch20130033	1
Hoffmann/ Noweda	Ethanol 96% pure / denatured	E-231213-1	3
BMV Branntwein	Ethanol 96% pure / denatured	Ch19	1
Hoffmann	Ethanol 96% pure / denatured	E-200412-1	3
Monopolstelle Jenne	Ethanol 96% pure / denatured	J150114	1
Merck	Ethanol 96% pure / denatured	K43729871232	3
Merck	Ethanol 96% pure / denatured	K44538471324	1
BFB	Ethanol 96% pure / denatured	keinevorhanden	2
Gehe	Ethanol 96% pure / denatured	LieferungMai2013	1
BfB-Betrieb München	Ethanol 96% pure / denatured		1
Taoasis/K	Ethanol 96% pure / denatured	VE30892-112552	1
Werner Hofmann	Ethanol 96% pure / denatured	8021304	1
PVL	Ethanol 96% pure / denatured	1204131	1
Bergchemie	Ethanol 96% pure / denatured	10/01/10	1
Noweda	Ethanol 96% pure / denatured	1202124	2
Bergchemie	Ethanol 96% pure / denatured	12/06/14	1
Berkel AHG	Ethanol 96% pure / denatured	12/11/23	1
Caelo	Ethanol 96% pure / denatured	12345	1
Berkel AHK	Ethanol 96% pure / denatured	1410T31141212	1
Klenk	Ethanol 96% pure / denatured	123456	1
Herbasin	Ethanol 96% pure / denatured	13/01/10	1
Laborch. Apolda	Ethanol 96% pure / denatured	18001881	1
Euro OTC	Ethanol 96% pure / denatured	18001042	1
Phönix/berkel	Ethanol 96% pure / denatured	130208	1
Gehe Laborchemie Apolda...	Ethanol 96% pure / denatured	19000689	1
Berkel AHK	Ethanol 96% pure / denatured	170412/292	1
Laborchemie Apolda GmbH...	Ethanol 96% pure / denatured	19000121	1
Berkel AHK	Ethanol 96% pure / denatured	1410T31080113	1
Laborchemie APOLDA GmgH	Ethanol 96% pure / denatured	19000689	1
Anzag	Ethanol 96% pure / denatured	19000121	1
Apolda / Gehe	Ethanol 96% pure / denatured	20000065	1
Laborchemie Apolda GmbH	Ethanol 96% pure / denatured	19001937	1
Laborchemie Apolda	Ethanol 96% pure / denatured	19001519	1
Bioenergie Icking	Ethanol 96% pure / denatured	201102170016	1
Schmittmann/Hoffmann	Ethanol 96% pure / denatured	20020112-1	1
Noweda	Ethanol 96% pure / denatured	19002422	2
Anzag 24.05.2012	Ethanol 96% pure / denatured	19000700	1
Werner Hofmann	Ethanol 96% pure / denatured	20150278	1
Caelo	Ethanol 96% pure / denatured		3
Applichem	Ethanol 96% pure / denatured	220113PML01	1
Berkel AHK	Ethanol 96% pure / denatured	2906211085	1
Hoffmann	Ethanol 96% pure / denatured	28081201	1
Fagron	Ethanol 96% pure / denatured		1
Caelo	Ethanol 96% pure / denatured	5678	1
Werner Hoffmann	Ethanol 96% pure / denatured		1
Gehe	Ethanol 96% pure / denatured	DE00001237810	1
sanacorp	Ethanol 96% pure / denatured	K40787471	1
Berkel AHK	Ethanol 96% pure / denatured	VE28587	1
Caelo	Ethanol 96% pure / denatured	K43619871227	1

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Supplier	Substance	Batch	Spectra
VDL	Ethanol 96% pure / denatured	K43005871151	1
Hersteller: Laborchemie...	Ethanol 96% pure / denatured	172N0346	1
Berkel	Ethanol 96% pure / denatured	1410T31260814	1
Noweda	Ethanol 96% pure / denatured	19001935	1
Werner Hofmann	Ethanol 96% pure / denatured	111111	1
Laborchemie / Noweda	Ethanol 96% pure / denatured	20001830	1
Laborchemie Apolda	Ethanol 96% pure / denatured	20001199	1
Phoenix	Ethanol 96% pure / denatured	200000973	1
Laborchemie Apolda	Ethanol 96% pure / denatured	20001885	1
Laborchemie	Ethanol 96% pure / denatured	21000152	1
spinnrad	Ethanol 96% pure / denatured	815310072	1
Brand GmbH Alkoholvertr...	Ethanol 96% pure / denatured	24052013/60	1
Agralko	Ethanol 96% pure / denatured	1062015	1
Kammer Kirschner	Ethanol 96% pure / denatured		3
Tereos/Berkel AHK	Ethanol 96% pure / denatured	31115/705	1
Bundes...	Ethanol 96% pure / denatured	8042014	1
Alkoholvertrieb Süd	Ethanol 96% pure / denatured	3297636/11062014	1
Alkoholvertrieb Süd/Gehe	Ethanol 96% pure / denatured	3297636/11062014	1
Schmittmann GmbH	Ethanol 96% pure / denatured	2041503	1
Apolda GmbH	Ethanol 96% pure / denatured	100050	1
Laborchemie Apolda/Jenn...	Ethanol 96% pure / denatured	12345	4
Berkel AHK	Ethanol 96% pure / denatured	120516/746	1
Werner Hoffmann	Ethanol 96% pure / denatured	7081503	1
Kottkamp/Anzag	Ethanol 96% pure / denatured	130116/505/020	1
Heyl / Sanacorp	Ethanol 96% pure / denatured		1
Berkel AHK	Ethanol 96% pure / denatured	14/01/30	1
Bergchemie	Ethanol 96% pure / denatured	14/02/27	1
Berkel AHK	Ethanol 96% pure / denatured	14/09/17	1
Berkel AHK	Ethanol 96% pure / denatured	14/10/16	1
/Phönix	Ethanol 96% pure / denatured	140604	1
Berkel AHK	Ethanol 96% pure / denatured	14/11/13	1
Berkel	Ethanol 96% pure / denatured	1410T31141015	1
Bergchemie	Ethanol 96% pure / denatured	14-06-04	1
Berkel AHK	Ethanol 96% pure / denatured	1410T31050914	1
Fagron	Ethanol 96% pure / denatured	1410T31200516	1
Berkel	Ethanol 96% pure / denatured	1410T31051115	1
Bundesm.Brandwein	Ethanol 96% pure / denatured	140710	1
BerkelAHK	Ethanol 96% pure / denatured	1410T31271115	1
Bergchemie	Ethanol 96% pure / denatured	14-10-16	1
Berkel AHK	Ethanol 96% pure / denatured	1410T31280116	1
Berkel AHK	Ethanol 96% pure / denatured	15/03/15	1
Berkel	Ethanol 96% pure / denatured	1410T31310715	1
bergchemie	Ethanol 96% pure / denatured	14-12-10	1
Berkel	Ethanol 96% pure / denatured	15/06/10	1
Bergchemie	Ethanol 96% pure / denatured	15/06/10	1
Berkel AHK	Ethanol 96% pure / denatured	15/07/23	2
Bergchemie	Ethanol 96% pure / denatured	15-05-07	1
Bergchemie	Ethanol 96% pure / denatured	16/01/06	2
Bergchemie	Ethanol 96% pure / denatured	15-10-09	1
Berkel AHK	Ethanol 96% pure / denatured	151125	1
Brüggemann	Ethanol 96% pure / denatured	1514041040	1
Bergchemie	Ethanol 96% pure / denatured	15-5-07	1
Bergchemie	Ethanol 96% pure / denatured	16/02/02	1
Bergchemie	Ethanol 96% pure / denatured	16/08/03	1
Hoffmann	Ethanol 96% pure / denatured	16061405	1
Kottkamp / über GEHE	Ethanol 96% pure / denatured	160714/505/004	1
Kassner & Sasse	Ethanol 96% pure / denatured	200-578-6	1
Fagron	Ethanol 96% pure / denatured	19001836	1
Apolda/Gehe	Ethanol 96% pure / denatured	20002193	1
Laborchemie Apolda	Ethanol 96% pure / denatured	17041401	1

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Supplier	Substance	Batch	Spectra
Caelo	Ethanol 96% pure / denatured	20001583	1
Eal Euro-Alkohol	Ethanol 96% pure / denatured	20140100	1
Schmittmann	Ethanol 96% pure / denatured	20150108	1
eal/euro-alkohol	Ethanol 96% pure / denatured	20150108	1
Agralko	Ethanol 96% pure / denatured	2015010901	1
Schmittmann GmbH	Ethanol 96% pure / denatured	20140100	1
Hoffmann/Schmittmann	Ethanol 96% pure / denatured	20150108	1
Euro Alkohol GmbH	Ethanol 96% pure / denatured	20150108	1
Caelo	Ethanol 96% pure / denatured	20150908	1
Hofmann/Schmittmann	Ethanol 96% pure / denatured	20160007	1
Laborchemie Apolda	Ethanol 96% pure / denatured	21000152	2
Apolda/ Sanacorp	Ethanol 96% pure / denatured	21000154	2
Noweda	Ethanol 96% pure / denatured	21000197	1
Noweda / Aploda	Ethanol 96% pure / denatured	21000197	1
Heyl / Sanacorp	Ethanol 96% pure / denatured	21001373	1
Laborchemie Apolda	Ethanol 96% pure / denatured	21001054	1
Phoenix	Ethanol 96% pure / denatured	21001561	1
Heyl / Sanacorp	Ethanol 96% pure / denatured	21001379	1
alliance Health. 23.10.14	Ethanol 96% pure / denatured	21001379	1
Apolda/ Sanacorp	Ethanol 96% pure / denatured	21001380	1
Apolda/ Sanacorp	Ethanol 96% pure / denatured	21001560	1
LaborchemieApolda/Sanac...	Ethanol 96% pure / denatured	21001053	1
Caelo	Ethanol 96% pure / denatured	21001964	1
Apolda GmbH	Ethanol 96% pure / denatured	21001382	1
Apolda GmbH	Ethanol 96% pure / denatured	21001379	2
Apolda gmbH/N	Ethanol 96% pure / denatured	21002064	1
Laborchemie Apolda über...	Ethanol 96% pure / denatured	21001964	1
Heyl(Laborchemie Apolda...	Ethanol 96% pure / denatured	21002064	1
Laborchemie Apolda	Ethanol 96% pure / denatured	21002075	3
Caelo	Ethanol 96% pure / denatured	21002244	1
Gehe/Dr. Wollff	Ethanol 96% pure / denatured	21002237	1
Phönix 06.2.15	Ethanol 96% pure / denatured	21002075	1
Apolda/ Sanacorp	Ethanol 96% pure / denatured	21002239	1
Laborchemie Apolda	Ethanol 96% pure / denatured	21002244	2
Sanacorp	Ethanol 96% pure / denatured	21002268	1
Noweda/laborchemie Apolda	Ethanol 96% pure / denatured	21002237	1
Laborch. Apolda/ Noweda	Ethanol 96% pure / denatured	21002237	1
Laborchemie Apolda GmbH	Ethanol 96% pure / denatured	21002268	1
Apolda/ Sanacorp	Ethanol 96% pure / denatured	22000090	1
Laborchemie Apolda/Phönix	Ethanol 96% pure / denatured	21002268	1
Fagron	Ethanol 96% pure / denatured	22000096	1
Apolda/Sanacorp	Ethanol 96% pure / denatured	22000090	1
Phoenix Goettin	Ethanol 96% pure / denatured	21002269	1
Laborchemie Apolda/Phönix	Ethanol 96% pure / denatured	22000392	1
Heyl/Noweda	Ethanol 96% pure / denatured	22000326	1
Apolda/Phönix	Ethanol 96% pure / denatured	21002269	1
Laborchemie/Noweda	Ethanol 96% pure / denatured	22000161	1
Laborchemie Apolda/Alli...	Ethanol 96% pure / denatured	22000392	1
Laborchemie Apolda/Gehe	Ethanol 96% pure / denatured	22000394	2
Laborchemie Apolda	Ethanol 96% pure / denatured	22000394	1
Heyl/ Gehe	Ethanol 96% pure / denatured	22000603	3
Laborchemie Apolda	Ethanol 96% pure / denatured	22000999	1
Caelo	Ethanol 96% pure / denatured	22000999	1
Apolda/Phönix	Ethanol 96% pure / denatured	22000616	1
Apolda/Phoenix	Ethanol 96% pure / denatured	22000616	1
Laborchemie Apolda GmbH.	Ethanol 96% pure / denatured	22000603	1
Laborchemie Apolda GmbH...	Ethanol 96% pure / denatured	22000616	1
Caelo	Ethanol 96% pure / denatured	22000641	1
Noweda 04.08.15	Ethanol 96% pure / denatured	22000616	1
Apolda gmbH/N	Ethanol 96% pure / denatured	22000999	1

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Supplier	Substance	Batch	Spectra
Laborchemie Apolda	Ethanol 96% pure / denatured	22001292	1
Laborchemie Apolda/Alli...	Ethanol 96% pure / denatured	22001291	1
Laborchemie Apolda/Sana...	Ethanol 96% pure / denatured	22000999	1
Laborchemie / Sanacorp	Ethanol 96% pure / denatured	22001717	1
Laborch. Apolda/ Noweda	Ethanol 96% pure / denatured	22001291	1
Laborchemie Apolda/Phönix	Ethanol 96% pure / denatured	22001291	1
Apolda/Phönix	Ethanol 96% pure / denatured	22001291	1
Laborchemie Apolda	Ethanol 96% pure / denatured	22001385	1
Apolda / Anzag	Ethanol 96% pure / denatured	22001717	1
Laborch. Apolda/ Noweda	Ethanol 96% pure / denatured	22001718	1
Caelo	Ethanol 96% pure / denatured	22001718	1
Apolda / Sanacorp	Ethanol 96% pure / denatured	22001985	1
Laborchemie Apolda über...	Ethanol 96% pure / denatured	22002230	1
Bionorica	Ethanol 96% pure / denatured	22001720	1
Laborchemie Apolda GmbH	Ethanol 96% pure / denatured	22001985	1
Gehe	Ethanol 96% pure / denatured	23000175	1
Laborchemie Apolda/ San...	Ethanol 96% pure / denatured	22002231	1
Caelo	Ethanol 96% pure / denatured	23000175	1
Laborchemie Apoldo GmbH	Ethanol 96% pure / denatured	22002231	1
Heyl	Ethanol 96% pure / denatured	23000188	1
Caelo	Ethanol 96% pure / denatured	23000480	1
Heyl/Noweda	Ethanol 96% pure / denatured	23000749	1
Caelo	Ethanol 96% pure / denatured	23000749	1
Laborch. Apolda/ Noweda	Ethanol 96% pure / denatured	23000997	1
Laborchemie Apolda/Phönix	Ethanol 96% pure / denatured	23001368	1
Laborchemie Apolda über...	Ethanol 96% pure / denatured	23000997	1
Apolda / Gehe	Ethanol 96% pure / denatured	23001357	1
Laborchemie Apolda/ All...	Ethanol 96% pure / denatured	23001368	1
Heyl / Noweda	Ethanol 96% pure / denatured	23001368	1
Rondell Apotheke	Ethanol 96% pure / denatured	410040216085	1
Kost/sophien	Ethanol 96% pure / denatured	410010414067	1
Kwst/Walther CMP	Ethanol 96% pure / denatured	290814	1
Hessische Spezialitäten...	Ethanol 96% pure / denatured	4101081501	1
Karl-Josef Kost Alkohol...	Ethanol 96% pure / denatured	41004115082	1
Miller Alkoholvertrieb ...	Ethanol 96% pure / denatured	410-103-150508/26052	1
Karl-Josef Kost Alkohol...	Ethanol 96% pure / denatured	410190516087	1
Brüggemann Alcohol	Ethanol 96% pure / denatured	7814070382	1
Merck	Ethanol 96% pure / denatured	45056971	1
Alkoholvertrieb Süd/DPD	Ethanol 96% pure / denatured	41010315061020072015	1
Brüggemann Alcohol	Ethanol 96% pure / denatured	7814120470	1
Brüggemann	Ethanol 96% pure / denatured	7815040634	1
Brüggeman Alkohol	Ethanol 96% pure / denatured	7815040634	1
Brüggemann	Ethanol 96% pure / denatured	7815030598	1
Brüggemann	Ethanol 96% pure / denatured	7815080789	2
Brüggemann	Ethanol 96% pure / denatured	7816041610	1
AgrAlko	Ethanol 96% pure / denatured	A2014000328	1
Kassner & Sasse/Apothek...	Ethanol 96% pure / denatured	A2013000183	2
Brüggemann	Ethanol 96% pure / denatured	7815110957	1
Bergchemie	Ethanol 96% pure / denatured	aaaaaa	1
Hoffmann/ Martinus-Apot...	Ethanol 96% pure / denatured	E-060815-1	1
Merck	Ethanol 96% pure / denatured	Index-No603-002-00-5	1
Merck	Ethanol 96% pure / denatured	K45475971416	3
Merck	Ethanol 96% pure / denatured	K45475971	1
Alfred Quadflieg, Gelse...	Ethanol 96% pure / denatured	K16/08/03	1
Merck	Ethanol 96% pure / denatured	K46405471507	2
Caelo	Ethanol 96% pure / denatured	K46109471	1
Brüggemann	Ethanol 96% pure / denatured	N781601257	1
Gehe Kassel	Ethanol 96% pure / denatured		1
Taosis / G	Ethanol 96% pure / denatured	VE31397-114015	1
Berkel AHK Alkoholhandel	Ethanol 96% pure / denatured	VE32507	1

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Supplier	Substance	Batch	Spectra
Berkel AHK	Ethanol 96% pure / denatured	VE37799	1
Berkel AHK Alkoholhandel	Ethanol 96% pure / denatured	VE32323	1
Gutenberg-Apotheke	Ethanol 96% pure / denatured	904214	1
Kottkamp Alkoholvertrie...	Ethanol 96% pure / denatured	160714/505/004	1
Kottkamp/Phönix	Ethanol 96% pure / denatured	151215/505/019	1
Laborchemie Apolda	Ethanol 96% pure / denatured	21000197	1
Apolda, direkt best.	Ethanol 96% pure / denatured	21001560	1
Laborchemie Apolda GmbH	Ethanol 96% pure / denatured	21001736	1
Laborchemie APOLDA GmbH	Ethanol 96% pure / denatured	21001561	1
Laborchemie Apolda ,Gehe	Ethanol 96% pure / denatured	21002075	1
Laborchemie Apolda GmbH	Ethanol 96% pure / denatured	21002269	1
Laborchemie APOLDA GmbH	Ethanol 96% pure / denatured	22000616	1
Apolda/Phönix	Ethanol 96% pure / denatured	22000096	1
Laborchemie Apolda ,Gehe	Ethanol 96% pure / denatured	22000641	1
Laborchemie APOLDA GmbH	Ethanol 96% pure / denatured	22001291	1
.....	Ethanol 96% pure / denatured	22001720	1
Apolda/Spangro	Ethanol 96% pure / denatured	22002231	1
Laborchemie Apolda GmbH	Ethanol 96% pure / denatured	22002231	1
Laborchemie Apolda GmbH	Ethanol 96% pure / denatured	23000188	1
Alkoholvertrieb Dr. Ber...	Ethanol 96% pure / denatured	41010414052992014	1
Caelo	Ethanol 96% pure / denatured	19002599	1
Apolda, Phönix	Ethanol 96% pure / denatured	20000307	1
A.H.D.	Ethanol 96% pure / denatured	20000305	1
Apolda GmbH/N/PZN:10137...	Ethanol 96% pure / denatured	20000975	1
Apolda, Gehe	Ethanol 96% pure / denatured	20001887	1
Apolda, Gehe	Ethanol 96% pure / denatured	20002192	1
Sanacorp	Ethanol 96% pure / denatured	20001830	1
	Ethanol 96% pure / denatured		1
Bundesmonopolstelle für...	Ethanol 96% pure / denatured	xxxx	2
Bundesmonopolverwaltung...	Ethanol 96% pure / denatured	2032012GI	1
Fiebig	Ethanol 96% pure / denatured	12020161/1	1
Kottkamp Alkoholvertrieb	Ethanol 96% pure / denatured	180213	1
Bergchemie	Ethanol 96% pure / denatured	5/0810	1
Caelo	Ethanol 96% pure / denatured	915A-03041	1
Post-Apotheke	Ethanol 96% pure / denatured	111a-02304	1
Berkel AHK	Ethanol 96% pure / denatured	91214/632	1
Berkel AHK	Ethanol 96% pure / denatured	1137111/08	1
Berkel AHK	Ethanol 96% pure / denatured	111016/786	1
Brüggemann	Ethanol 96% pure / denatured	1514020991	1
BERKEL AHK	Ethanol 96% pure / denatured	170712/334	4
Laborchemie Apolda/Jenn...	Ethanol 96% pure / denatured	20002191	1
Berkel AHK /TEREOS	Ethanol 96% pure / denatured	190515/669	1
Lamotte/PX	Ethanol 96% pure / denatured	200201121	1
eal	Ethanol 96% pure / denatured	20150108	1
Hofmann	Ethanol 96% pure / denatured	20150278	1
Laborchemie Apolda	Ethanol 96% pure / denatured	21001380	1
Berkel AHK	Ethanol 96% pure / denatured	200214/567	1
Karl-Josef Kost	Ethanol 96% pure / denatured	410040216085	1
Berkel AHK	Ethanol 96% pure / denatured	210714/598	1
Hofmann,Branntweinmonopol	Ethanol 96% pure / denatured	20140162	1
Laborchemi Apolda	Ethanol 96% pure / denatured	22000395	1
Sophien-AM / K.J.Kost	Ethanol 96% pure / denatured	410041115082	1
AgrAlko	Ethanol 96% pure / denatured	410-1405	1
Berkel AHK	Ethanol 96% pure / denatured	60919/1La	1
Merck	Ethanol 96% pure / denatured		1
Sanacorp	Ethanol 96% pure / denatured		1
Spinnrad	Ethanol 96% pure / denatured	713310072	1
Hofmann,Branntweinmonopol	Ethanol 96% pure / denatured		2
Werner Hofmann	Ethanol 96% pure / denatured	20120106	1
Berkel	Ethanol 96% pure / denatured	1410T31191113	1

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Supplier	Substance	Batch	Spectra
Berkel AHK	Ethanol 96% pure / denatured	1410T31181213	1
Berkel AHK	Ethanol 96% pure / denatured	13/09/05	2
Caelo	Ethanol 96% pure / denatured	20001887	1
BfB	Ethanol 96% pure / denatured	10065927	1
Werner Hoffmann	Ethanol 96% pure / denatured	20130033	1
Caelo	Ethanol 96% pure / denatured	AKD7	1
eal Euro-Alkohol	Ethanol 96% pure / denatured		1
Klenk	Ethanol 96% pure / denatured	10059387-15102	1

- 57 990 spectra from 332 *Apo-Ident* customers from a total of 19 810 batches from a further 328 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 96% pure / denatured* 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 96% pure / denatured* 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	34 264
Type B	0	80	0	63 414
Type C	0	426	25	57 967

The substance/substance group *Ethanol 96% pure / denatured* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5967 %)	94.4568 % (> 93.7916 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31488	31488	0.00	53.49
31564	31488	4.37	50.44

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Ethyl acetate**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30719-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Ethyl acetate; Aether aceticus; Ethylis acetas

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Ethyl acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ethyl acetate	11357003	30719	40	1402681
Caelo	Ethyl acetate	13366102	31385	40	20131107

Validation samples

A total of 156 379 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 *Ethyl acetate*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 1 reference samples from the substance/substance group *Ethyl acetate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ethyl acetate	15362301	32568	40

- 63 554 spectra from a total of 1476 batches from further 439 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 9 *Apo-Ident* customers from 7 batches from the substance/substance group *Ethyl acetate*.

Supplier	Substance	Batch	Spectra
Caelo	Ethyl acetate	15362301	1
Caelo	Ethyl acetate	9081304	1
Caelo	Ethyl acetate	13366101	1
Caelo	Ethyl acetate	11357003	2
Caelo	Ethyl acetate	10286201	1
Caelo	Ethyl acetate	15182402	2
Caelo	Ethyl acetate	12357601	1

- 58 432 spectra from 332 *Apo-Ident* customers from a total of 20 085 batches from a further 328 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 *Ethyl acetate* 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 *Ethyl acetate* 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	34 264
Type B	0	40	0	63 554
Type C	0	9	0	58 432

The substance/substance group *Ethyl acetate* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.5973 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30719	30719	0.00	56.05
31385	30719	8.91	48.72

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Eucalyptus oil / Rosmary oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30875-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Eucalyptus oil / Rosmary oil; Eucalypti aetheroleum; Eucalyptus oil; Oleum eucalypti; Oleum rosmarini; Rosemary oil; Rosmarini aetheroleum

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Eucalyptus oil / Rosmary oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Rosemary oil	12E08-N05	30875	40	1502124
Bombastus	Eucalyptus oil	279796	31110	40	73399
Caelo	Eucalyptus oil	13106314	31284	34	AR-15-FG-000909-01

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Eucalyptus oil	14039604	31285	38	1412280
Caelo	Eucalyptus oil	14039609	31298	40	20140214
Euro OTC	Rosemary oil	1303016-01	31311	40	1502125
Caelo	Eucalyptus oil	14121904	31314	40	AR-15-FG-004302-01
Euro OTC	Eucalyptus oil	1406028-01	31527	40	20140716
Euro OTC	Rosemary oil	1511016	31822	40	20151214*
Euro OTC	Eucalyptus oil	1511015	31823	40	20151214*
Caelo	Eucalyptus oil	14039626	31864	40	20140211
Caelo	Eucalyptus oil	15316504	31865	40	20150925

Validation samples

A total of 156379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 472 spectra of 12 reference samples from the substance/substance group *Eucalyptus oil* / *Rosemary oil*. These samples are listed above in the [calibration samples](#) section.
- 33872 spectra from a total of 786 batches from further 223 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 340 spectra of 11 reference samples from the substance/substance group *Eucalyptus oil* / *Rosemary oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Eucalyptus oil	92752399	30253	40
Caelo	Eucalyptus oil	11104312	30859	40
Euro OTC	Eucalyptus oil	1406028-01	31527 [†]	20
Euro OTC	Rosemary oil	1511016	31822 [†]	20
Euro OTC	Eucalyptus oil	1511015	31823 [†]	20
Caelo	Eucalyptus oil	14039626	31864 [†]	20
Caelo	Eucalyptus oil	15316504	31865 [†]	20
Caelo	Rosemary oil	162769	32686	40
Euro OTC	Eucalyptus oil	1608042	32773	40
Euro OTC	Rosemary oil	1608043	32774	40
Caelo	Eucalyptus oil	163513	33084	40

*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.

- 63 254 spectra from a total of 1466 batches from further 438 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.

- 377 spectra from 126 *Apo-Ident* customers from 200 batches from the substance/substance group *Eucalyptus oil* / *Rosmary oil*.

Supplier	Substance	Batch	Spectra
Caelo	Eucalyptus oil	13106326	3
Caelo	Eucalyptus oil	1214E-01978	1
Fagron	Eucalyptus oil	13E15-N04	3
Caelo	Eucalyptus oil	14039609	11
Caelo	Eucalyptus oil	14039602	1
Caelo	Eucalyptus oil	14039625	3
Fagron	Eucalyptus oil	14A17-B40	1
Bombastus	Eucalyptus oil	293175	1
Bombastus	Eucalyptus oil	286454	1
Euro OTC	Eucalyptus oil	1211028-02	2
Fagron	Eucalyptus oil	11D11-N02	1
Fagron	Eucalyptus oil	192680-0002	1
Bombastus	Eucalyptus oil	269495	1
Caelo	Eucalyptus oil	916M-01978	1
Fagron	Eucalyptus oil	11K23-N05	2
Fagron	Eucalyptus oil	12G25-N11	4
Caelo	Eucalyptus oil	12114112	5
Frey & Lau GmbH/Phoenix	Eucalyptus oil	12G25-N11	1
Caelo	Eucalyptus oil	13106411	3
Caelo	Eucalyptus oil	13106403	3
Caelo	Eucalyptus oil	13106412	3
Caelo	Eucalyptus oil	13106413	1
Caelo	Eucalyptus oil	14039604	1
Caelo	Eucalyptus oil	14039601	2
Caelo	Eucalyptus oil	14039603	1
ahd/lamotte	Eucalyptus oil	14039604	1
Caelo	Eucalyptus oil	14039618	3
Caelo	Eucalyptus oil	14039610	1
Caelo	Eucalyptus oil	14039622	2
Caelo	Eucalyptus oil	14039626	7
Gehe 20.02.15	Eucalyptus oil	1406028-02	1
Caelo	Eucalyptus oil	14039627	1
Caelo	Eucalyptus oil	14121904	5
Phönix	Eucalyptus oil	14A17-B40	2
Fagron	Eucalyptus oil	14A17-B40-291551	1
Caelo	Eucalyptus oil	1439603	1
Phönix	Eucalyptus oil	14A17-B40-291551	1
Fagron	Eucalyptus oil	14e09-b06-294679	1
Fagron	Eucalyptus oil	14E09-B06-294681	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
phönix	Eucalyptus oil	14E09-B06-294681	1
Caelo	Eucalyptus oil	15011701	1
Caelo	Eucalyptus oil	15011704	1
Caelo	Eucalyptus oil	15063302	1
Caelo	Eucalyptus oil	15063303	1
Caelo	Eucalyptus oil	15063301	1
Caelo	Eucalyptus oil	15063309	7
Caelo	Eucalyptus oil	15063312	5
Caelo	Eucalyptus oil	1515Q-01978	1
Caelo	Eucalyptus oil	15316501	2
Caelo	Eucalyptus oil	15316502	3
Caelo	Eucalyptus oil	15316512	1
Caelo	Eucalyptus oil	15316504	2
Caelo	Eucalyptus oil	15400202	2
Caelo	Eucalyptus oil	15400203	1
Fagron	Eucalyptus oil	15B03-B02-304362	2
Caelo	Eucalyptus oil	28071502	1
Bombastus	Eucalyptus oil	286740	2
Bombastus	Eucalyptus oil	285615	1
Bombastus	Eucalyptus oil	288085	3
Bombastus	Eucalyptus oil	290094	1
Bombastus	Eucalyptus oil	291597	1
Caelo	Eucalyptus oil	292087	1
Bombastus	Eucalyptus oil	293087	2
Bombastus	Eucalyptus oil	299699	1
Sanacorp	Eucalyptus oil		2
Sanacorp	Eucalyptus oil	48/AKD3	1
Bombastus	Eucalyptus oil	293227	1
Bombastus	Eucalyptus oil	294687	1
Caelo	Eucalyptus oil	4136096	1
Bombastus	Eucalyptus oil	298889	1
Caelo	Eucalyptus oil	296079	1
Taoasis	Eucalyptus oil	8745-115428	1
Bombastus	Eucalyptus oil	296079	1
Caelo	Eucalyptus oil	513I-01978	1
Taoasis	Eucalyptus oil	8745-116747	1
Caelo	Eucalyptus oil	9351601	1
Caelo	Eucalyptus oil	10051816	1
Caelo	Eucalyptus oil	7011302	1
Caelo	Eucalyptus oil	10318506	1
Euro OTC	Eucalyptus oil	110801001	1
ANZAG 19.12.2012	Eucalyptus oil	110801001	1
Fagron	Eucalyptus oil	11102506	1
Caelo	Eucalyptus oil	11102507	2
Caelo	Eucalyptus oil	11324107	6
Caesar & Loretz GmbH D-...	Eucalyptus oil	11102507	1
Caelo	Eucalyptus oil	11324108	1
Caelo	Eucalyptus oil	11324112	8
Caelo	Eucalyptus oil	12103605	1
Euro OTC	Eucalyptus oil	1202030-01	1
Caelo	Eucalyptus oil	12103607	3
Caelo	Eucalyptus oil	12103611	4
Euro OTC	Eucalyptus oil	1211028-01	2
Caelo	Eucalyptus oil	12103612	1
Caelo	Eucalyptus oil	12114107	2
Caelo	Eucalyptus oil	12114111	1
PVL	Eucalyptus oil	1260813	1
Fagron	Eucalyptus oil	12B23-N08	6
Euro OTC	Eucalyptus oil	12D05-N03	1
Fagron	Eucalyptus oil	12D05-N03	1

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Supplier	Substance	Batch	Spectra
Caelo	Eucalyptus oil	13106401	4
Caelo	Eucalyptus oil	13106301	1
Spirig/Noweda	Eucalyptus oil	13106401	2
Caelo	Eucalyptus oil	13106304	1
Caelo	Eucalyptus oil	13106402	2
Noveda	Eucalyptus oil	13106402	1
Caelo	Eucalyptus oil	14a17-b40-29155	1
Caelo	Eucalyptus oil	2112I-01978	1
Bombastus	Eucalyptus oil	261706	1
Bombastus	Eucalyptus oil	270004	1
Caelo	Eucalyptus oil	270421	1
Bombastus	Eucalyptus oil	273707	1
Caelo	Eucalyptus oil	275646	1
Anzag 14.06.2013	Eucalyptus oil	275484	1
Anzag	Eucalyptus oil	273707	1
Bombastus	Eucalyptus oil	276113	1
Bombastus	Eucalyptus oil	275646	1
Bombastus	Eucalyptus oil	278619	1
Euro OTC	Eucalyptus oil	278619	2
Bombastus	Eucalyptus oil	279798	1
Bombastu-Werke AG/Gehe	Eucalyptus oil	282165	1
Caelo	Eucalyptus oil	3012E-01978	1
AHD 03.12.2013	Eucalyptus oil	282165	1
Taoasis GmbH	Eucalyptus oil	33364-110969	1
Bombastus	Eucalyptus oil	285362	2
Bombastus	Eucalyptus oil	283384	1
Bombastu-Werke AG/Gehe	Eucalyptus oil	283991	1
Taoasis	Eucalyptus oil	502745-108325	1
Bombastus	Eucalyptus oil	284861	1
Taoasis	Eucalyptus oil	53970-110969	1
Taoasis	Eucalyptus oil	527885-109905	1
Taoasis	Eucalyptus oil	521399-108557	1
Taoasis	Eucalyptus oil	543495-112704	1
Taoasis	Eucalyptus oil	557095-114030	1
Gehe 12.04.2013	Eucalyptus oil		1
Caelo	Eucalyptus oil		1
Bergland / Gehe	Eucalyptus oil	K301874	1
Bergland / Gehe	Eucalyptus oil	K302509	1
Bombastus	Eucalyptus oil		2
Caelo	Eucalyptus oil	13106316	2
Caelo	Eucalyptus oil	14039612	1
Caelo	Eucalyptus oil	15316507	1
Bombastus	Eucalyptus oil	281667	1
Bomastus direkt	Eucalyptus oil	293624	1
Fagron	Rosemary oil	12E08-N05	4
Fagron	Rosemary oil	13I19-B04	2
Caelo	Rosemary oil	2613M-02012	1
Bombastus	Rosemary oil	296037	1
Bombastus	Rosemary oil	282541	1
Caelo	Rosemary oil	1209034-01	2
Euro OTC	Rosemary oil	1209034-01	2
Euro OTC	Rosemary oil	1202025-01	2
Caelo	Rosemary oil	12246517	1
Caelo	Rosemary oil	12246501	5
Caelo	Rosemary oil	11287208	4
Fagron	Rosemary oil	13B18-N01	3
Bombastus	Rosemary oil	281945	1
Bergland/Sanacorp	Rosemary oil	C301101-3448311132	1
Euro OTC	Rosemary oil	1404037-01	1
Bombastus	Rosemary oil	288951	1

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Supplier	Substance	Batch	Spectra
Bombastus	Rosemary oil	295093	1
Bombastus	Rosemary oil	273724	3
Caelo	Rosemary oil	11031402	1
Caelo	Rosemary oil	12246520	2
Fagron	Rosemary oil	13/19-B04-293577	4
Frey & Lau GmbH/Phoenix	Rosemary oil	13/19-B04-293575	1
Caelo	Rosemary oil	13/19-B04-293577	3
Fagron	Rosemary oil	13/19-B04-308855	1
Euro OTC	Rosemary oil	130801401	2
Phönix	Rosemary oil	131119-B04	1
Fagron	Rosemary oil	13I19-B04-293577	2
Fagron	Rosemary oil	13I19B04	1
Euro OTC	Rosemary oil	1404037-02	1
Caelo	Rosemary oil	13I19-B04-293599	1
Caelo	Rosemary oil	14092910	1
Caelo	Rosemary oil	14092904	1
Caelo	Rosemary oil	14092911	1
Bombastus	Rosemary oil	285668	1
Caelo	Rosemary oil	296036	1
Bombastus	Rosemary oil	278770	1
Taoasis	Rosemary oil	26057-118014	1
Bombastus	Rosemary oil	2872889	1
Caelo	Rosemary oil	18091402	1
Caelo	Rosemary oil	31031502	1
Taoasis	Rosemary oil	3231031-117639	1
noweda	Rosemary oil		1
Caelo	Rosemary oil	3091206	1
Caelo	Rosemary oil	4101301	1
PVL	Rosemary oil	491212	1
Noweda	Rosemary oil	10374817	1
Caelo	Rosemary oil	10374817	2
Hedinger	Rosemary oil	11287208	1
Caelo	Rosemary oil	11287211	6
Anzag 05.11.12 ek:7,37	Rosemary oil	11287211	1
Noweda	Rosemary oil	11287211	1
Fagron	Rosemary oil	11K21-N05	3
Noweda	Rosemary oil	11287211ui	1
Taoasis	Rosemary oil	121217-110772	1
Caelo	Rosemary oil	12236401	1
Caelo	Rosemary oil	12246508	6
Anzag 12.03.13 ek: 7,37EUR	Rosemary oil	12246508	1
Fagron	Rosemary oil	12246508	1
AHD , 03.09.13	Rosemary oil	12246515	2
Caelo	Rosemary oil	12246515	3
Gehe 14.06.2013	Rosemary oil	12G12-N12	1
Fagron	Rosemary oil	13/19-B04-287289	1
Taoasis	Rosemary oil	130313-111912	1
Euro OTC	Rosemary oil	1303016-01	1
Fagron	Rosemary oil	13A28-N03	3
Taoasis GmbH	Rosemary oil	130815-113178	1
fargo	Rosemary oil	13A28-N03	2
Großhandel	Rosemary oil	13A28-N03	1
Caelo	Rosemary oil	1511016-01	1
Euro OTC	Rosemary oil	1511016-02	1
Caelo	Rosemary oil	15316704	1
Caelo	Rosemary oil	17012014	1
Caelo	Rosemary oil	15442017	1
Caelo	Rosemary oil	2715E-02012	1
Caelo	Rosemary oil	273098	1
phönix 14.08.2013	Rosemary oil	275963	1

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Supplier	Substance	Batch	Spectra
Caelo	Rosemary oil	275963	1
Caelo	Rosemary oil	278907	2
Bombastus	Rosemary oil	278907	2
Caelo	Rosemary oil	279984	1
Caelo	Rosemary oil	28051309	1
Phönix	Rosemary oil	282665	1
Euro OTC	Rosemary oil	290203901	1
Taoasis GmbH	Rosemary oil	3231016-115522	1
Fagron	Rosemary oil	693655-N12	1
Taoasis GmbH	Rosemary oil	7028-105285	1

- 58 064 spectra from 332 *Apo-Ident* customers from a total of 19 895 batches from a further 327 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 *Eucalyptus oil* / *Rosemary oil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Eucalyptus oil* / *Rosemary oil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	472	0	33 872
Type B	0	320	20	63 254
Type C	0	357	20	58 064

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9689 %)	100.0000 % (> 98.7288 %)
Type B	100.0000 % (> 99.9710 %)	94.1176 % (> 93.2353 %)
Type C	100.0000 % (> 99.5963 %)	94.6950 % (> 93.8992 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30875	30875	0.00	42.16
31110	31823	4.85	40.23
31284	31284	0.00	40.58
31285	31285	0.00	38.88
31298	31285	1.49	38.48
31311	31311	0.00	40.91
31314	31314	0.00	40.12
31527	31823	3.12	38.30
31822	31822	0.00	41.51
31823	31823	0.00	40.72
31864	31823	2.35	40.53
31865	31314	5.93	42.13

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Eugenol**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31286-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Eugenol; Eugenolum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Eugenol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Eugenol	13401501	31286	40	1407436
Caelo	Eugenol	13401506	31397	40	20131213

Validation samples

A total of 156 379 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 *Eugenol*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 1 reference samples from the substance/substance group *Eugenol*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Eugenol	15H11-B03-322946	32731	40

- 63 554 spectra from a total of 1476 batches from further 439 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 *Eugenol*.

Supplier	Substance	Batch	Spectra
Caelo	Eugenol	14165403	1
Caelo	Eugenol	15255901	1
Caelo	Eugenol	15255904	1
Caelo	Eugenol	14165401	1

- 58 437 spectra from 332 *Apo-Ident* customers from a total of 20 088 batches from a further 328 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 *Eugenol* 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 *Eugenol* 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	34 264
Type B	0	40	0	63 554
Type C	0	3	1	58 437

The substance/substance group *Eugenol* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.5985 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31286	31286	0.00	40.66
31397	31286	1.62	42.74

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Fennel honey (conserved)
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30900-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fennel honey (conserved); Mel foeniculi (konserviert)

Special notes

When selecting the *Fennel honey (conserved)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 honey (conserved)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fennel honey (co...	12247203	30900	40	1402574
Caelo	Fennel honey (co...	14045202	31598	40	20140317

Validation samples

A total of 156 379 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 *Fennel honey (conserved)*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Fennel honey (conserved)*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fennel honey (conserved)	12247203	30900 [†]	20
Caelo	Fennel honey (conserved)	14045202	31598 [†]	20

- 63 554 spectra from a total of 1475 batches from further 439 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 honey (conserved)*.

Supplier	Substance	Batch	Spectra
Caelo	Fennel honey (conserved)	13152605	1

[†]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*.

- 58 440 spectra from 332 *Apo-Ident* customers from a total of 20 091 batches from a further 328 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 honey (conserved)* 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 honey (conserved)* 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	34 264
Type B	0	34	6	63 554
Type C	0	1	0	58 440

The substance/substance group *Fennel honey (conserved)* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	85.0000 % (> 77.5000 %)
Type C	100.0000 % (> 99.6053 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30900	30900	0.00	17.20
31598	30900	10.47	22.93

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Fennel oil, bitter
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30398-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fennel oil, bitter; Oleum foeniculi amari

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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, bitter*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fennel oil, bitter	14190402	31706	40	20140625
Caelo	Fennel oil, bitter	15160103	31805	40	1703170
Bombastus	Fennel oil, bitter	295236	32922	40	1704221

Validation samples

A total of 156 379 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 *Fennel oil, bitter*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 160 spectra of 5 reference samples from the substance/substance group *Fennel oil, bitter*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fennel oil, bitter	9366708	30169	40
Bombastus	Fennel oil, bitter	264987	30398	40
Caelo	Fennel oil, bitter	14190402	31706 [†]	20
Caelo	Fennel oil, bitter	15160103	31805 [†]	20
Caelo	Fennel oil, bitter	16008606	32961	40

- 63 434 spectra from a total of 1472 batches from further 439 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 19 *Apo-Ident* customers from 16 batches from the substance/substance group *Fennel oil, bitter*.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Fennel oil, bitter	24101403	1
Caelo	Fennel oil, bitter	12218103	4
Erika Apotheke	Fennel oil, bitter	12218104	1
Caelo	Fennel oil, bitter	15160101	1
Caelo	Fennel oil, bitter	12218104	5
Caelo	Fennel oil, bitter	12370303	1
Caelo	Fennel oil, bitter	12061412	1
Caelo	Fennel oil, bitter	12370306	3
Caelo	Fennel oil, bitter	12370312	2
Celo / Kehr	Fennel oil, bitter	12370314	1
Bombastus	Fennel oil, bitter	291598	1
Bombastus	Fennel oil, bitter	278909	3
Caelo	Fennel oil, bitter	268017	1
Sanacorp	Fennel oil, bitter	278909	1
Bombastus	Fennel oil, bitter	289232	1
Bombastus	Fennel oil, bitter	281715	1
Bombastus	Fennel oil, bitter	274253	1
Bombastus	Fennel oil, bitter	285544	1

- 58 411 spectra from 332 *Apo-Ident* customers from a total of 20 076 batches from a further 328 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, bitter* 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, bitter* 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	34 224
Type B	0	130	30	63 434
Type C	0	25	5	58 411

The substance/substance group *Fennel oil, bitter* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9710 %)	81.2500 % (> 79.3750 %)
Type C	100.0000 % (> 99.5966 %)	83.3333 % (> 73.3333 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31706	31805	1.59	63.50
31805	31805	0.00	63.23
32922	32922	0.00	46.01

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Formic acid 85%**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30591-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Formic acid 85%; Acidum formicicum 85%; Acidum formicicum crudum 85%

Special notes

When selecting the *Formic acid 85%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Formic acid 85%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Formic acid 85%	11194901	30591	40	1402561
Caelo	Formic acid 85%	13373301	31320	40	20131118

Validation samples

A total of 156379 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 *Formic acid 85%*. These samples are listed above in the [calibration samples](#) section.
- 34264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 20 spectra of 1 reference samples from the substance/substance group *Formic acid 85%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Formic acid 85%	13373301	31320 [†]	20

- 63574 spectra from a total of 1476 batches from further 439 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 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Formic acid 85%*.

Supplier	Substance	Batch	Spectra
Caelo	Formic acid 85%	10343801	1
Hedinger	Formic acid 85%	170912	1
Anzag/ Fischar	Formic acid 85%		1
Hedinger	Formic acid 85%	383338	1

[†]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*.

- 58 437 spectra from 332 *Apo-Ident* customers from a total of 20 089 batches from a further 328 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 *Formic acid 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 *Formic acid 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	80	0	34 264
Type B	0	20	0	63 574
Type C	0	4	0	58 437

The substance/substance group *Formic acid 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9712 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.5985 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30591	30591	0.00	394.67
31320	30591	4.26	398.98

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Gel Cordes®**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30632-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Gel Cordes®

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Gel Cordes®*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Ichthyol	Gel Cordes®	12A035	30632	40	1405096
Ichthyol	Gel Cordes®	13A007	31083	40	20130513
Ichthyol	Gel Cordes®	15A099	31876	40	20150624
Ichthyol	Gel Cordes®	15A099	32911	40	20150624

Validation samples

A total of 156379 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 *Gel Cordes*[®]. These samples are listed above in the [calibration samples](#) section.
- 34184 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 136 spectra of 5 reference samples from the substance/substance group *Gel Cordes*[®].

Supplier	Substance	Batch	Sample ID	Spectra
Ichthyol	Gel Cordes [®]	14A017	30714	40
Ichthyol	Gel Cordes [®]	15A099	31876 [†]	20
Ichthyol	Gel Cordes [®]	15A099	32910	40
Ichthyol	Gel Cordes [®]	15A099	not required	24
Ichthyol	Gel Cordes [®]	16A169	not required	12

- 63458 spectra from a total of 1474 batches from further 439 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 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Gel Cordes*[®].

Supplier	Substance	Batch	Spectra
Ichthyol/Anzag	Gel Cordes [®]	12A035	2

continued on the next page

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

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Supplier	Substance	Batch	Spectra
Noweda/Ichthyol-Gesells...	Gel Cordes [®]	14A017	3
Ichthyol/Alliance Healt...	Gel Cordes [®]	15A099	3
Caelo	Gel Cordes [®]	13A007	2
Noweda/Ichthyol-Gesells...	Gel Cordes [®]	15A099	1
Ichthyol/Gehe	Gel Cordes [®]	15A099	1
Cordes GmbH/Noweda	Gel Cordes [®]	15A099	2

- 58 427 spectra from 332 *Apo-Ident* customers from a total of 20 088 batches from a further 328 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 *Gel 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 *Gel 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	160	0	34 184
Type B	0	96	40	63 458
Type C	0	14	0	58 427

The substance/substance group *Gel 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	70.5882 % (> 68.3824 %)
Type C	100.0000 % (> 99.5969 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30632	30632	0.00	41.08
31083	30632	15.50	39.54
31876	30632	15.98	39.89
32911	30632	12.19	39.81

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Geranium oil, genuine
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30468-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Geranium oil, genuine; Oleum geranii verum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Geranium oil, genuine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Geranium oil, ge...	12354109	31193	40	1403533
Caelo	Geranium oil, ge...	15172205	31789	40	20150608

Validation samples

A total of 156 379 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 *Geranium oil, genuine*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Geranium oil, genuine*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Geranium oil, genuine	11275601	30468	40
Caelo	Geranium oil, genuine	15172205	31789 [†]	20

- 63 534 spectra from a total of 1475 batches from further 439 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 *Geranium oil, genuine*.

Supplier	Substance	Batch	Spectra
Caelo	Geranium oil, genuine	11275605	1
Caelo	Geranium oil, genuine	16070403	1
Caelo	Geranium oil, genuine	35434343	1

[†]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*.

- 58 438 spectra from 332 *Apo-Ident* customers from a total of 20 089 batches from a further 328 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 *Geranium oil, genuine* 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 *Geranium oil, genuine* 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	34 264
Type B	0	60	0	63 534
Type C	0	3	0	58 438

The substance/substance group *Geranium oil, genuine* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.5993 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31193	31193	0.00	75.98
31789	31193	4.89	74.51

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Glucose syrup
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30934-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glucose syrup; Glucose syrup GE 40%; Glucosum liquidum; Sirupus Glucosi

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Glucose syrup*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Glucose syrup	12I18-N11	30934	40	1403229
Fagron	Glucose syrup	14G16-T01-018036	31603	40	20150120

Validation samples

A total of 156 379 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 *Glucose syrup*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 100 spectra of 3 reference samples from the substance/substance group *Glucose syrup*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Glucose syrup	14G16-T01-018036	31603 [†]	20
Fagron	Glucose syrup	14G16-T01-018036	32272	40
Fagron	Glucose syrup	16B02-T11-029595	32273	40

- 63 494 spectra from a total of 1475 batches from further 439 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 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Glucose syrup*.

Supplier	Substance	Batch	Spectra
Fagron	Glucose syrup	13D23-N02	1
Fagron	Glucose syrup	10J25-T52-013485	1

continued on the next page

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

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Supplier	Substance	Batch	Spectra
Phönix	Glucose syrup	13D23-N02	1
Fagron	Glucose syrup	13G03-N01	2

- 58 436 spectra from 332 *Apo-Ident* customers from a total of 20 089 batches from a further 328 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 *Glucose syrup* 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 *Glucose syrup* 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	34 264
Type B	0	100	0	63 494
Type C	0	5	0	58 436

The substance/substance group *Glucose syrup* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.5981 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30934	30934	0.00	27.57
31603	30934	6.65	28.86

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Glycerine ointment (conserved)**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30986-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Glycerine ointment (conserved); Glyceroli unguentum (konserviert); Unguentum glycerini (konserviert)

Special notes

When selecting the *Glycerine ointment (conserved)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Glycerine ointment (conserved)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glycerine ointme...	12288201	30986	40	20121017
Caelo	Glycerine ointme...	14031701	31296	40	1410452

Validation samples

A total of 156379 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 *Glycerine ointment (conserved)*. These samples are listed above in the [calibration samples](#) section.
- 34264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Glycerine ointment (conserved)*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glycerine ointment (conserved)	16192001	32589	40
Caelo	Glycerine ointment (conserved)	17049101	33240	40

- 63514 spectra from a total of 1475 batches from further 439 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 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Glycerine ointment (conserved)*.

Supplier	Substance	Batch	Spectra
Caelo	Glycerine ointment (conserved)	13250102	2
Caelo	Glycerine ointment (conserved)	14183401	5
Caelo	Glycerine ointment (conserved)	15025101	2

- 58 432 spectra from 332 *Apo-Ident* customers from a total of 20 089 batches from a further 328 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 *Glycerine ointment (conserved)* 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 *Glycerine ointment (conserved)* 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	34 264
Type B	0	80	0	63 514
Type C	0	9	0	58 432

The substance/substance group *Glycerine ointment (conserved)* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5973 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30986	31296	10.94	35.23
31296	31296	0.00	36.14

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Glycerol >99%**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30189-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Glycerol >99%; Glycerinum anhydricum >99%

Special notes

When selecting the *Glycerol >99%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Glycerol >99%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glycerol >99%	12111504	30871	40	20120418
Caelo	Glycerol >99%	13127603	31152	40	1405278
Caelo	Glycerol >99%	13370502	31352	40	20131115
Caelo	Glycerol >99%	162308	32693	40	20160809*

Validation samples

A total of 156 379 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 *Glycerol* >99%. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 189 spectra of 4 reference samples from the substance/substance group *Glycerol* >99%.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glycerol >99%	10198706	30189	89
Caelo	Glycerol >99%	10198706	30231	40
Caelo	Glycerol >99%	13370502	31352 [†]	20
Caelo	Glycerol >99%	162308	32325	40

- 63 405 spectra from a total of 1474 batches from further 439 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.

- 224 spectra from 97 *Apo-Ident* customers from 48 batches from the substance/substance group *Glycerol* >99%.

*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.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Glycerol >99%	13127610	2
Caelo	Glycerol >99%	13370502	6
Caelo	Glycerol >99%	13370503	13
Caelo	Glycerol >99%	14373403	12
Caelo	Glycerol >99%	14373409	7
Caelo	Glycerol >99%	14373413	19
Beiersdorf AG	Glycerol >99%	15406501	1
Caelo	Glycerol >99%	1474303	1
Caelo	Glycerol >99%	15406501	9
Caelo	Glycerol >99%	16023504	11
Caelo	Glycerol >99%	11217403	1
Caelo	Glycerol >99%	11305101	1
Caesar & Lorenz	Glycerol >99%	13002904	1
Caelo	Glycerol >99%	13111403	1
Caelo	Glycerol >99%	4031501	1
Caelo	Glycerol >99%	13127604	10
Caelo	Glycerol >99%	13127608	5
Caelo	Glycerol >99%	13370501	2
Phönix	Glycerol >99%	13127610	1
Caelo	Glycerol >99%	133370507	1
Caelo	Glycerol >99%	14074302	10
Gehe 16.12.14	Glycerol >99%	13370503	1
Caelo	Glycerol >99%	13370507	1
Caesar & Loretz GmbH Hi...	Glycerol >99%	14074302	1
Caelo	Glycerol >99%	14074303	2
Caelo	Glycerol >99%	14373401	1
Caesar & Loretz GmbH	Glycerol >99%	14373403	1
Caelo	Glycerol >99%	14373404	2
Fagron	Glycerol >99%	14373409	2
Noweda	Glycerol >99%	14373413	1
Caelo	Glycerol >99%	15283603	1
Caelo	Glycerol >99%	15406502	5
Caelo	Glycerol >99%	15406503	2
Phoenix	Glycerol >99%	16023504	2
Caelo	Glycerol >99%	16023503	1
Caelo	Glycerol >99%	15406504	2
Caelo	Glycerol >99%	17041403	1
Caelo	Glycerol >99%	16023506	2
Caesar & Loretz GmbH Hi...	Glycerol >99%	16023506	1
Caelo	Glycerol >99%	510211590	1
Caelo	Glycerol >99%	18081504	1
Caelo	Glycerol >99%	2114Q1590	1
Caelo	Glycerol >99%	2061201	1
Caelo	Glycerol >99%	11061303	1
Caelo	Glycerol >99%	1004211590	1
Caelo	Glycerol >99%	11118104	1
Caelo	Glycerol >99%	11305102	2
Phönix 22.08.12	Glycerol >99%	11305102	1
Caelo	Glycerol >99%	12014304	14
Gehe	Glycerol >99%	12014304	1
Caelo	Glycerol >99%	12111503	5
Caelo	Glycerol >99%	12111504	3
Gehe	Glycerol >99%	12111504	2
Caelo	Glycerol >99%	13002903	7
Caelo	Glycerol >99%	13002902	1
Caelo	Glycerol >99%	12111505	1
Caelo	Glycerol >99%	13002904	5
Fagron	Glycerol >99%	13002904	1
Gehe	Glycerol >99%	13002904	1
Phönix	Glycerol >99%	13002904	2

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Supplier	Substance	Batch	Spectra
Caelo	Glycerol >99%	1300291	1
Caelo	Glycerol >99%	13127603	17
Caelo	Glycerol >99%	2713M1590	1
Gehe	Glycerol >99%	13127603	2
apomix/ Phoenix	Glycerol >99%	13127608	2
Caesar & Loretz GmbH Hi...	Glycerol >99%	13127608	1
Caelo	Glycerol >99%	1317604	1
Phönix/EuRho	Glycerol >99%	12111503	2

- 58 217 spectra from 332 *Apo-Ident* customers from a total of 20 044 batches from a further 328 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 *Glycerol >99%* 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 *Glycerol >99%* 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	34 184
Type B	0	189	0	63 405
Type C	0	222	2	58 217

The substance/substance group *Glycerol >99%* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 96.8254 %)
Type C	100.0000 % (> 99.5963 %)	99.1071 % (> 97.7679 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30871	31152	4.05	97.94
31152	31152	0.00	100.45
31352	31152	4.32	93.94
32693	32693	0.00	161.84

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Glycerol 85%
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30886-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glycerol 85%; Glycerinum 85%; Glycerolum 85%

Special notes

When selecting the *Glycerol 85%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Glycerol 85%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glycerol 85%	12216606	30886	70	20120731
Fagron	Glycerol 85%	12H16-N04	30980	80	20120905
Caelo	Glycerol 85%	13356404	31360	40	20131112
Caelo	Glycerol 85%	13406202	31377	40	20131219
Euro OTC	Glycerol 85%	1409035-01	31588	40	AR-15-FG-007030-02
Euro OTC	Glycerol 85%	1506036	31719	40	0000010478
Euro OTC	Glycerol 85%	1509023	31737	40	20151005*
Euro OTC	Glycerol 85%	1601059	31956	40	20160225*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 390 spectra of 8 reference samples from the substance/substance group *Glycerol 85%*. These samples are listed above in the [calibration samples](#) section.
- 33 954 spectra from a total of 790 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 470 spectra of 15 reference samples from the substance/substance group *Glycerol 85%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glycerol 85%	12216606	30886 [†]	10
Caelo	Glycerol 85%	13356404	31360 [†]	20
Euro OTC	Glycerol 85%	1409035-01	31588 [†]	20
Euro OTC	Glycerol 85%	1506036	31719 [†]	20
Euro OTC	Glycerol 85%	1509023	31737 [†]	20
Euro OTC	Glycerol 85%	1601059	31956 [†]	20
Caelo	Glycerol 85%	160637	32203	40
Caelo	Glycerol 85%	160637	32314	40
Caelo	Glycerol 85%	162153	32326	40
Caelo	Glycerol 85%	162189	32328	40
Caelo	Glycerol 85%	162978	32694	40
Euro OTC	Glycerol 85%	1607037	32703	40
Euro OTC	Glycerol 85%	1610032	32828	40
Caelo	Glycerol 85%	163550	33097	40
Caelo	Glycerol 85%	163472	33098	40

- 63 124 spectra from a total of 1463 batches from further 439 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the

*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.

[†]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*.

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.

- 1383 spectra from 262 *Apo-Ident* customers from 380 batches from the substance/substance group *Glycerol 85%*.

Supplier	Substance	Batch	Spectra
Caelo	Glycerol 85%	11217302	2
Caelo	Glycerol 85%	11324201	3
Caelo	Glycerol 85%	12108201	21
Caelo	Glycerol 85%	465911	1
Lamotte//AHD	Glycerol 85%	125545	1
Hedinger/Phönix	Glycerol 85%	40513	1
Hedinger / Gehe	Glycerol 85%	40515	1
Hedinger/Phoenix	Glycerol 85%	40515	1
Hedinger/Noweda	Glycerol 85%	40515	1
Hedinger	Glycerol 85%	40519	3
Euro OTC	Glycerol 85%	40524	1
Hedinger	Glycerol 85%	40531	2
Phönix/Hedinger	Glycerol 85%	40524	1
Hedinger	Glycerol 85%	40524	1
Hedinger/Gehe	Glycerol 85%	40529	2
Stumpf/Hedinger	Glycerol 85%	40531	1
Hedinger	Glycerol 85%	40538	1
Hedinger/Gehe	Glycerol 85%	40540	1
Hedinger/Phoenix	Glycerol 85%	40542	1
Hedinger	Glycerol 85%	40548	2
Hedinger/Sanacorp	Glycerol 85%	40548	2
Hedinger/PX	Glycerol 85%	40547	1
Caelo	Glycerol 85%	40556	1
Caelo	Glycerol 85%	40542	3
Hedinger	Glycerol 85%	40556	2
Stumpf / Hedinger	Glycerol 85%	40557	1
Hedinger	Glycerol 85%	40557	2
August Hedinger	Glycerol 85%	40557	1
Hedinger/ Noweda	Glycerol 85%	40574	1
Hedinger/Noweda	Glycerol 85%	40574	1
Hedinger/ Sanacorp	Glycerol 85%	40567	1
Hedinger	Glycerol 85%	40566	3
Hedinger/Phönix	Glycerol 85%	40559	1
Hedinger	Glycerol 85%	40576	2
Rondell Apotheke	Glycerol 85%	40576	1
Heedinger/Noweda	Glycerol 85%	40576	1
Hedinger/Sanacorp	Glycerol 85%	40579	1
Hedinger/Phoenix	Glycerol 85%	40579	1
Hedinger/ Sanacorp	Glycerol 85%	40584	2
Phoenix	Glycerol 85%	40596	1
Hedinger/ Sanacorp	Glycerol 85%	40599	2
Hedinger	Glycerol 85%	40598	1
Hedinger/Phoenix	Glycerol 85%	40596	1
Jenne	Glycerol 85%	40599	1
Hedinger	Glycerol 85%	40586	1
Caelo	Glycerol 85%	40607	1
Fischar/ Gehe	Glycerol 85%	1076011	1

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Supplier	Substance	Batch	Spectra
Caelo	Glycerol 85%	8121402	1
otto fischer	Glycerol 85%	1075111	1
Caelo	Glycerol 85%	5051501	1
Hedinger	Glycerol 85%	40599	1
Caelo	Glycerol 85%	11355301	1
Caelo	Glycerol 85%	12216601	8
Caelo	Glycerol 85%	13144604	7
Caelo	Glycerol 85%	13144606	6
noweda	Glycerol 85%	13276202	1
Caelo	Glycerol 85%	13276024	1
Caelo	Glycerol 85%	13276202	1
Caelo	Glycerol 85%	13276203	12
Caelo	Glycerol 85%	13276204	13
Caelo	Glycerol 85%	13276205	20
noweda	Glycerol 85%	13356403	1
Caelo	Glycerol 85%	13356403	2
Caelo	Glycerol 85%	13356404	11
Caelo	Glycerol 85%	13356405	10
Gehe	Glycerol 85%	13356405	1
Phönix	Glycerol 85%	13356406	1
Caelo	Glycerol 85%	13356406	7
Caelo	Glycerol 85%	13406202	6
Caelo	Glycerol 85%	13406203	1
Caelo	Glycerol 85%	13406204	6
Fagron	Glycerol 85%	13J01-B01-285781	2
Caelo	Glycerol 85%	13406205	2
Euro OTC	Glycerol 85%	1401009-01	8
Euro OTC	Glycerol 85%	1403006-01	4
Fagron	Glycerol 85%	13J29-B01-285782	1
Euro OTC	Glycerol 85%	14050021-02	1
Euro OTC	Glycerol 85%	1405021-01	3
Euro OTC	Glycerol 85%	1409035-01	10
Euro OTC	Glycerol 85%	1405021-02	3
Caelo	Glycerol 85%	14148103	3
Caelo	Glycerol 85%	1409035-01	2
Caelo	Glycerol 85%	14149403	19
Phönix	Glycerol 85%	14149403	1
Ph.Eur.7.0	Glycerol 85%	14148106	1
Caelo	Glycerol 85%	14148105	1
Caelo	Glycerol 85%	14149404	8
Caelo	Glycerol 85%	14148106	1
Caelo	Glycerol 85%	14149406	8
Caelo	Glycerol 85%	14149410	11
Sanacorp	Glycerol 85%	14149410	1
Caelo	Glycerol 85%	14149411	7
Caelo	Glycerol 85%	1419411	1
Caelo	Glycerol 85%	1418103	1
Caelo	Glycerol 85%	14194911	1
Caelo	Glycerol 85%	14249301	2
Fagron	Glycerol 85%	14306202	2
Caelo	Glycerol 85%	14306202	1
Caelo	Glycerol 85%	14306203	13
Caelo	Glycerol 85%	14306204	7
Euro OTC	Glycerol 85%	1502010-01	9
Caelo	Glycerol 85%	1502010-01	1
Bombastus	Glycerol 85%	1502010-01	1
Caelo	Glycerol 85%	15036901	1
Sanacorp	Glycerol 85%	15036902	1
Caelo	Glycerol 85%	15036902	10
Caelo	Glycerol 85%	15036903	9

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Supplier	Substance	Batch	Spectra
Phoenix	Glycerol 85%	15036903	1
Caelo	Glycerol 85%	15036904	9
Caelo	Glycerol 85%	15036905	2
Caelo	Glycerol 85%	15050102	6
Caelo	Glycerol 85%	15049801	2
Caelo	Glycerol 85%	15050101	1
Euro OTC	Glycerol 85%	1506036-01	6
Caelo	Glycerol 85%	15115005	1
Caelo	Glycerol 85%	15146304	1
Caelo	Glycerol 85%	1514604	1
Caelo	Glycerol 85%	15146305	1
Bombastus	Glycerol 85%	15146303	1
Caelo	Glycerol 85%	15283504	1
Caelo	Glycerol 85%	15283505	1
Caelo	Glycerol 85%	1528503	1
Caelo	Glycerol 85%	1529201	1
Caelo	Glycerol 85%	15292201	8
Caelo	Glycerol 85%	15292202	7
Caelo	Glycerol 85%	15292203	5
Caelo	Glycerol 85%	15292204	11
Caelo	Glycerol 85%	15292205	9
Sanacorp	Glycerol 85%	15292205	2
Caelo	Glycerol 85%	15378202	4
Caelo	Glycerol 85%	15378203	4
Caelo	Glycerol 85%	15379201	2
Caelo	Glycerol 85%	16063701	8
Caelo	Glycerol 85%	15378210	1
Caelo	Glycerol 85%	16215301	3
Caelo	Glycerol 85%	15404505	2
Caesar & Loretz GmbH Hi...	Glycerol 85%	16063702	1
Caelo	Glycerol 85%	16063702	6
Phönix	Glycerol 85%	15378203	2
Bombastus	Glycerol 85%	284400	5
Caelo	Glycerol 85%	16215310	1
Caelo	Glycerol 85%	17061404	1
Bombastus	Glycerol 85%	285366	2
Caelo	Glycerol 85%	2714M-01589	1
Bombastus	Glycerol 85%	293387	2
Gehe	Glycerol 85%	287120	2
Bombastus	Glycerol 85%	289295	3
Bombastus	Glycerol 85%	292791	8
Eigenherstellung	Glycerol 85%	295501	1
Bombastus	Glycerol 85%	291085	3
Bombastus	Glycerol 85%	295501	4
Bombastus	Glycerol 85%	296481	1
2959	Glycerol 85%	2959	1
Bombastus	Glycerol 85%	294927	3
Bombastus	Glycerol 85%	300393	1
Bombastus	Glycerol 85%	300394	1
Fischar	Glycerol 85%	5063091	1
Bombastus	Glycerol 85%	298592	2
Fischar	Glycerol 85%	5055031	1
Nowed 18.12.2014	Glycerol 85%		2
Caelo	Glycerol 85%	5015Q-01589	1
fischar gmbh	Glycerol 85%	5064011	1
Fischar	Glycerol 85%	5063092	1
Fischer	Glycerol 85%	5063091	1
fischar gmbh	Glycerol 85%	5064021	1
Fischar/V.d.L.	Glycerol 85%	5064071	1
Fischar	Glycerol 85%	5065011	1

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Supplier	Substance	Batch	Spectra
Caelo	Glycerol 85%	5064091	1
Fischar/ Now	Glycerol 85%	5065011	1
Fischar / Phönix	Glycerol 85%	5065031	2
Herbeta Arzneimittel Be...	Glycerol 85%		1
Fischar/ Now	Glycerol 85%	5065111	2
Lamotte	Glycerol 85%	5603001	7
Jenne/Lamotte	Glycerol 85%	5603001	1
Lamotte	Glycerol 85%	5538401	7
Test	Glycerol 85%	Test	1
Henry Lamotte	Glycerol 85%	5603001	1
Lamotte	Glycerol 85%	5603002	1
Caelo	Glycerol 85%	271511	1
Noweda	Glycerol 85%	272305	1
Henry Lamotte	Glycerol 85%	123142	1
Sanacorp	Glycerol 85%	273719	1
Caelo	Glycerol 85%	123142	2
Lamotte	Glycerol 85%	123142	1
Lamotte	Glycerol 85%	123304	4
Bombastus	Glycerol 85%	272305	3
Henry	Glycerol 85%	123304	2
Lamotte	Glycerol 85%	123464	5
Henry Lamotte	Glycerol 85%	123304	1
Sanacorp/ Heddinge	Glycerol 85%	400473	2
Hedinger Jenne	Glycerol 85%	40462	1
Hedinger	Glycerol 85%	40464	2
Hedinger	Glycerol 85%	40471	2
Hedinger Phönix	Glycerol 85%	40471	1
Hedinger	Glycerol 85%	40473	1
Anzag/ Hedinger	Glycerol 85%	40478	1
Hedinger/Gehe	Glycerol 85%	40473	1
Anzag/Seeger	Glycerol 85%	40475	2
Sanacorp	Glycerol 85%	40480	1
Hedinger/ Sanacorp	Glycerol 85%	40479	2
Großhandel	Glycerol 85%	40473	1
Anzag/Seeger	Glycerol 85%	40483	2
Hedinger/ Anzag	Glycerol 85%	40491	1
Hedinger	Glycerol 85%	40483	2
Caelo	Glycerol 85%	40481	1
Caelo	Glycerol 85%	40483	1
Hedinger	Glycerol 85%	40497	4
Hedinger	Glycerol 85%	40506	2
Sanacorp	Glycerol 85%	40495	1
Phoenix	Glycerol 85%	40495	2
Hedinger/Phönix	Glycerol 85%	40501	1
Phönix/Hedinger	Glycerol 85%	40497	1
Sanacorp	Glycerol 85%	40506	1
Caelo	Glycerol 85%	40507	1
Hedinger	Glycerol 85%	40507	1
Hedinger	Glycerol 85%	40509	1
Caelo	Glycerol 85%	607211589	1
Bartel/Sanacorp	Glycerol 85%	40515	1
Caelo	Glycerol 85%	613Q-01589	1
Caelo	Glycerol 85%	1113E-01589	1
Europharm/Otto	Glycerol 85%	1108032-01	1
Caelo	Glycerol 85%	11217303	1
Caelo	Glycerol 85%	11324202	2
Caelo	Glycerol 85%	11L06-N02	4
Euro OTC	Glycerol 85%	120103801	1
Caelo	Glycerol 85%	11355305	1
Gehe	Glycerol 85%	1201038-01	1

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Supplier	Substance	Batch	Spectra
Anzag 17.09.2012	Glycerol 85%	12069603	1
Caelo	Glycerol 85%	12069601	2
Euro OTC	Glycerol 85%	1201038-01	9
Caelo	Glycerol 85%	12069604	1
Gehe 08.05.2013	Glycerol 85%	1210047-01	1
Noweda	Glycerol 85%	12108201	2
Fagron	Glycerol 85%	1209C001	1
Anzag/	Glycerol 85%	12108201	1
Caelo	Glycerol 85%	12069605	1
Phönix	Glycerol 85%	12108201	2
Caelo	Glycerol 85%	12108206	1
Phönix 15.12.12	Glycerol 85%	12216601	1
Caelo	Glycerol 85%	12216602	6
Caelo	Glycerol 85%	12216603	17
Caelo	Glycerol 85%	12216604	3
Caelo	Glycerol 85%	12216606	13
GEHE	Glycerol 85%	12216606	2
Gehe 25.04.2013	Glycerol 85%	12216606	1
Caelo	Glycerol 85%	12273604	24
Geo-Chem/sanacorp	Glycerol 85%	12216606	1
Phönix	Glycerol 85%	12273604	2
Phoenix	Glycerol 85%	12273604	1
Fagron	Glycerol 85%	12G11-N02	1
Fagron	Glycerol 85%	12H17-N01	2
Caelo	Glycerol 85%	12278507	2
A.H. 18.06.13 ek: 6,78EUR	Glycerol 85%	12273604	1
Caelo	Glycerol 85%	12278508	4
Fagron	Glycerol 85%	12J04-N02	1
Fagron	Glycerol 85%	12J04-N09	2
Fagron	Glycerol 85%	12J05-N01	1
Caelo	Glycerol 85%	13039202	5
Caelo	Glycerol 85%	13039204	21
Caelo	Glycerol 85%	13039203	17
Caelo	Glycerol 85%	13060001	5
Phönix 14.01.2014	Glycerol 85%	13060001	1
Caelo	Glycerol 85%	13060006	5
Fagron	Glycerol 85%	13060006	1
Caelo	Glycerol 85%	13060007	5
PHOENIX am 14.01.2014	Glycerol 85%	13060007	1
Euro OTC	Glycerol 85%	1306016-02	7
Caelo	Glycerol 85%	1309202	1
Caelo	Glycerol 85%	13144605	18
Caelo	Glycerol 85%	13144607	18
Gehe	Glycerol 85%	13144607	2
Caelo	Glycerol 85%	13248201	12
Caelo	Glycerol 85%	13248204	2
Fagron	Glycerol 85%	13C28-N02	9
Fagron	Glycerol 85%	13D11-N05	1
Fagron	Glycerol 85%	13C-N02	1
Fagron	Glycerol 85%	13E24-N11	3
Fagron	Glycerol 85%	13J29-B01	1
Phoenix	Glycerol 85%	1405021-01	1
Caelo	Glycerol 85%	140113PML02	1
Caelo	Glycerol 85%	14101304	1
Sanacorp	Glycerol 85%		2
Caelo	Glycerol 85%	2405211589	1
Phönix/	Glycerol 85%	14149410	1
Caelo	Glycerol 85%	2/AKD52	1
Caelo	Glycerol 85%	2413Q01589	1
Caelo	Glycerol 85%	16121301	1

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Supplier	Substance	Batch	Spectra
Caelo	Glycerol 85%	24021402	1
Caesar/Noweda	Glycerol 85%	2611I-01589	1
Caelo	Glycerol 85%	23081201	1
Bombastus	Glycerol 85%	275075	3
Bombastus	Glycerol 85%	278655	1
Kehr / Lamotte	Glycerol 85%	290114PML04	1
Bombastus	Glycerol 85%	276850	2
Hedinger/Gehe	Glycerol 85%	3112Q-01589	1
Bombastus	Glycerol 85%	282731	5
Gehe	Glycerol 85%	282731	1
Caelo	Glycerol 85%	4711A-01589	1
Caelo	Glycerol 85%	5x12273604	1
Kehr / Fischar	Glycerol 85%	5061071	1
Otto Fischar GmbH	Glycerol 85%	5061101	1
Fischar/E	Glycerol 85%	5062011	1
Caelo	Glycerol 85%	5x13039203	1
Gehe	Glycerol 85%	5062051	1
Caelo	Glycerol 85%	5062052	1
Otto Fischar/Gehe	Glycerol 85%	5063012	1
Otto Fischar GmbH	Glycerol 85%	5062052	4
Fischar	Glycerol 85%	5062111	4
Phönix	Glycerol 85%	5062111	1
Henry Lamotte	Glycerol 85%	5226901	2
Lamotte	Glycerol 85%	5360201	5
Henry Lamotte GmbH Bremen	Glycerol 85%	5142501	1
Lamotte	Glycerol 85%	5424901	4
Lamotte	Glycerol 85%	5424101	2
Lamotte	Glycerol 85%	5487801	2
Lamotte	Glycerol 85%	5512001	2
Krieger/14.04.14	Glycerol 85%	5538401	4
Caelo	Glycerol 85%		2
Hedinger	Glycerol 85%	40486	1
Hedinger/ Sanacorp	Glycerol 85%	40501	1
Hedinger	Glycerol 85%	40578	1
hedinger	Glycerol 85%	40494	1
Hedinger/ Sanacorp	Glycerol 85%	40499	1
heidringer	Glycerol 85%	40559	1
Caelo	Glycerol 85%	11324208	1
Caesar & Loretz GmbH	Glycerol 85%	12108201	1
Phoenix	Glycerol 85%	13039203	2
Fagron	Glycerol 85%	1312B03285613	1
Herbeta / Noweda	Glycerol 85%		2
Bombastus	Glycerol 85%	279852	3
Hedinger/Phönix	Glycerol 85%	40481	1
Hedinger/Phönix	Glycerol 85%	40531-1	1
Caelo	Glycerol 85%	13136115	1
Caelo	Glycerol 85%	13276208	4
Herbeta Berlin	Glycerol 85%		1
Otto Fischar GmbH/Anzag	Glycerol 85%	5064011	3
Hedinger Phönix	Glycerol 85%	40507	1
Fischar GmbH/AHD	Glycerol 85%	5064091	1
Caelo	Glycerol 85%	13276201	1
Caelo	Glycerol 85%	P136/14	1
Caelo	Glycerol 85%	40480	2
Hedinger/Phönix	Glycerol 85%	40483	2
Hedinger Phönix	Glycerol 85%	40495	1
Hedinger/Sanacorp	Glycerol 85%	40499-3354319071	1
Hedinger Jenne	Glycerol 85%	40501	1
Sanacorp	Glycerol 85%	278655	1
Sanacorp	Glycerol 85%	280855	2

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Supplier	Substance	Batch	Spectra
Caelo	Glycerol 85%	1309204	1
Noweda	Glycerol 85%	40475	2
Lamotte/Phönix	Glycerol 85%	124654	2
Alliance Health 27.11.2...	Glycerol 85%		1
Bombastus	Glycerol 85%	40215PJK01	1
Henry Lamotte	Glycerol 85%	124654	1
Hedinger/ Noweda	Glycerol 85%	40515	1
Sanacorp/ Hedinger	Glycerol 85%	40502	1
Hedinger/Gehe	Glycerol 85%	40519	1
Hedinger	Glycerol 85%	40502	1
Hedinger/Noweda	Glycerol 85%	40522	1
Hedinger/Gehe	Glycerol 85%	40524	1
hedinger/Gehe	Glycerol 85%	40529	1
Caelo	Glycerol 85%	40524	1
Hedinger	Glycerol 85%	40528	1
Caelo	Glycerol 85%	40529	1
Hedinger/Noweda	Glycerol 85%	40531	1
Hedinger/ Sanacorp	Glycerol 85%	40531-1	1
Hedinger	Glycerol 85%	40531-1	1
Caelo	Glycerol 85%	40540	1
Hedinger/ Sanacorp	Glycerol 85%	40538	1
HirschApotheke	Glycerol 85%	40541	1
Hedinger/Noweda	Glycerol 85%	40542	1
Hedinger	Glycerol 85%	40541	1
Hedinger/ Sanacorp	Glycerol 85%	40546	2
Hedinger/Phoenix	Glycerol 85%	40546	1
Hedinger/Phönix	Glycerol 85%	40546	1
Hedinger/Sanacorp	Glycerol 85%	40557	1
Hedinger/Noweda	Glycerol 85%	40559	2
Hedinger/ Sanacorp	Glycerol 85%	40559	1
Hedinger/Phoenix	Glycerol 85%	40559	1
Hedinger/Sanacorp	Glycerol 85%	40566	1
Hedinger	Glycerol 85%	40567	3
Hedinger/Noweda	Glycerol 85%	40566	1
Stumpf/Hedinger	Glycerol 85%	40576	1
Hedinger/Noweda	Glycerol 85%	40583	1
Hedinger/Sanacorp	Glycerol 85%	40576	1
Hedinger	Glycerol 85%	40579	1
Hedinger/Gehe	Glycerol 85%	40584	1
Hedinger	Glycerol 85%	40583	2
Hedinger	Glycerol 85%	40584	2
Hedinger/Noweda	Glycerol 85%	40586	1
Hedinger/Gehe	Glycerol 85%	40586	1
Hedinger/Noweda	Glycerol 85%	40599	1
Phoenix	Glycerol 85%	40586	1
GEHE 14.04.2014	Glycerol 85%	13276205	2
Cealo	Glycerol 85%	13276205	1
Sanacorp	Glycerol 85%	13276205	1
Caelo	Glycerol 85%	13276206	1
Caelo	Glycerol 85%	13356402	1
Caelo	Glycerol 85%	135406204	1
AHD	Glycerol 85%	13406202	1
Caelo	Glycerol 85%	13396407	1
Fagron	Glycerol 85%	13J01-B01	1
Fagron	Glycerol 85%	13J01-B01-285777	1
Euro OTC	Glycerol 85%	1401009	1
Euro OTC	Glycerol 85%	140502101	2
Caelo	Glycerol 85%	1404024-01	1
Caelo	Glycerol 85%	1405021	1
Gehe	Glycerol 85%	1405021-02	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Glycerol 85%	140903501	1
Caelo	Glycerol 85%	14148104	3
Gehe	Glycerol 85%	14149404	1
Caelo	Glycerol 85%	14306205	4
Gehe,06.05.15	Glycerol 85%	14306205	1
Euro OTC	Glycerol 85%	14380504	1
Fagron	Glycerol 85%	14A10-B01-291983	1
Fagron	Glycerol 85%	14D25-B02-293384	1
Caleo	Glycerol 85%	15036903	1
Euro OTC	Glycerol 85%	1509023-01	4
Caelo	Glycerol 85%	15146301	2
Caelo	Glycerol 85%	15146303	1
Phönix Gotha	Glycerol 85%	15146301	1
Caelo	Glycerol 85%	15283506	1
Caesar & Loretz GmbH Hi...	Glycerol 85%	15292204	1
Caelo	Glycerol 85%	15378201	1
Caelo	Glycerol 85%	153782019	1
Caelo	Glycerol 85%	15378209	1
Caelo	Glycerol 85%	15379207	2
Caelo	Glycerol 85%	15404504	2
Caesar & Loretz/Noweda	Glycerol 85%	15379208	1
Euro OTC	Glycerol 85%	1601059-01	6
Euro OTC	Glycerol 85%	160703701	1
Bombastus	Glycerol 85%	1607037-01	1
Caelo	Glycerol 85%	16063706	1
Caelo	Glycerol 85%	16215302	3
Bombastus	Glycerol 85%	2823731	1
otto fischer	Glycerol 85%	23081604	1
Bombastus	Glycerol 85%	260914PAS01	1
Hedinger	Glycerol 85%	25082015B	1
Perrigo/Phönix	Glycerol 85%	284401	1
Caelo	Glycerol 85%	24101401	1
Bombastus	Glycerol 85%	287120	1
Bombastus	Glycerol 85%	287890	1
Bombastus	Glycerol 85%	289296	1
Bombastus	Glycerol 85%	290715	1
Bombastus	Glycerol 85%	296480	1
Bombastus	Glycerol 85%	301816	2
Bombastus	Glycerol 85%	295502	1
Bombastus	Glycerol 85%	301817	2
Bombastus	Glycerol 85%	298593	1
Bombastus	Glycerol 85%	302750	2
Fischar	Glycerol 85%	5062012	4
Alliance Healthcare/Fis...	Glycerol 85%	5063011	1
Caelo	Glycerol 85%	5064021	1
Fischar / Phönix	Glycerol 85%	5064011	1
Otto Fischar	Glycerol 85%	5065012	1
Fischar/Phönix	Glycerol 85%	5064071	1
Otto Fischer	Glycerol 85%	5064011	1
Otto Fischar GmbH & Co...	Glycerol 85%	5065012	1
Noweda/ Fischar	Glycerol 85%	5065011	1
Fischar	Glycerol 85%	5065061	2
fischar	Glycerol 85%	5065061	2
Caelo	Glycerol 85%	5065061	1
Noweda/ Fischar	Glycerol 85%	5065061	2
Fischar / Alliance Hea...	Glycerol 85%	5065111	1
Otto Fischer	Glycerol 85%	5065081	1
Fischar/Gehe	Glycerol 85%	5065081	1
Fischar/ Phönix	Glycerol 85%	5065101	1
Fischar	Glycerol 85%	5066011	1

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Supplier	Substance	Batch	Spectra
Fischar / Noweda	Glycerol 85%	50655081	1
Otto Fischar GmbH/ Noweda	Glycerol 85%	5066011	4
Fischar / Phönix	Glycerol 85%	5066031	1
Fischar/ Now	Glycerol 85%	5066031	1
Alliance Healthcare	Glycerol 85%	5066061	1
Fischar	Glycerol 85%	5066071	1
Noweda	Glycerol 85%	5066071	1
Fischar/ Now	Glycerol 85%	5066071	4
fischar/Phönix	Glycerol 85%	5066071	1
Fischar	Glycerol 85%	5066031	1
Fischar/ Phönix	Glycerol 85%	5066081	1
Gehe/Fischar	Glycerol 85%	5066071	1
Henry Lamotte Oils	Glycerol 85%	5538401	6
fischar/Phönix	Glycerol 85%	50666061	1
Alliance Health 24.06.2...	Glycerol 85%	5538401	1
Henry Lamotte Oils	Glycerol 85%	5603001	5
noweda	Glycerol 85%		1
Sanacorp	Glycerol 85%	72/AKD1	1
Fagron	Glycerol 85%	56-81-5	1
Henry Lamotte Oils GmbH	Glycerol 85%	5603001	1
Caelo	Glycerol 85%	73/AKD2	1
Otto	Glycerol 85%		1
Pharmachem GmbH	Glycerol 85%	272305	4
Lamotte/AHD	Glycerol 85%	8001116001	1
Henry Lamotte Phönix	Glycerol 85%	123142	1
Bartel	Glycerol 85%	40475	2
Hedinger/Noweda	Glycerol 85%	40478	2
Heddinger/Sanacorp	Glycerol 85%	40475	2
Hedinger	Glycerol 85%	40480	1
Hedinger/ Sanacorp	Glycerol 85%	40480	2
Lamotte/Noweda	Glycerol 85%	123464	1
Phönix	Glycerol 85%	40481	1
Hedinger	Glycerol 85%	40478	1
Henry Lamotte	Glycerol 85%	123464	2
Henry Lamotte/Jenne	Glycerol 85%	123464	1
Hedinger/Noweda	Glycerol 85%	40480	1
Hedinger	Glycerol 85%	40481	1
hedinger	Glycerol 85%	40483	2
Hedinger/Ebert	Glycerol 85%	40483	1
Hedinger/Gehe	Glycerol 85%	40491	1
Gehe	Glycerol 85%	40491	2
Noweda/Hedinger	Glycerol 85%	40499	1
Hedinger/Gehe	Glycerol 85%	40497	2
Hedinger	Glycerol 85%	40499	4
Phönix	Glycerol 85%	40501	1
hedinger/Gehe	Glycerol 85%	40501	1
Großhandel	Glycerol 85%	40507	1
Hedinger/Noweda	Glycerol 85%	40502	1
Phönix	Glycerol 85%	40507	1
Caelo	Glycerol 85%	40515	1
Hedinger/Gehe	Glycerol 85%	4091	1
Caelo	Glycerol 85%	70913Gly	1
Euro OTC	Glycerol 85%	1210047-01	10
Gehe	Glycerol 85%	1210047-01	1
Caelo	Glycerol 85%	1213E-01589	1
Gehe 10.04.2013	Glycerol 85%	1227360	1
Caelo	Glycerol 85%	12278502	1
Caelo	Glycerol 85%	12278501	1
Euro OTC	Glycerol 85%	1301025-01	8
EuRho	Glycerol 85%	1301025-01	4

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Supplier	Substance	Batch	Spectra
Gehe	Glycerol 85%	1301025-01	1
Euro OTC	Glycerol 85%	1301025-02	2
Euro OTC	Glycerol 85%	1306016-01	2
Caelo	Glycerol 85%	13060002	2
Gehe	Glycerol 85%	1306016-02	1
Caelo	Glycerol 85%	1309203	1
Caesar & Loretz GmbH Hi...	Glycerol 85%	13144607	1
Fagron	Glycerol 85%	13c28-n02	2
Fagron	Glycerol 85%	250214PJK01	1
Caelo	Glycerol 85%	2013A-01589	1
Bombastus	Glycerol 85%	276852	4
Gehe	Glycerol 85%	276852	1
Bombastus	Glycerol 85%	2812731	2
Otto Fischar GmbH	Glycerol 85%	5062012	1
fischer, Gehe	Glycerol 85%	5062051	1
Bombastus	Glycerol 85%	280855	1
Fischar/Anzag	Glycerol 85%	5062111	1
Gehe	Glycerol 85%	5062121	1
Fischar/V.d.L.	Glycerol 85%	5062111	1
Otto Fischer GmbH	Glycerol 85%	5062121	3
Fischar	Glycerol 85%	5062121	1
Fischar	Glycerol 85%	5063011	2
Otto Fischar/Phoenix	Glycerol 85%	5063011	1
Gehe	Glycerol 85%	5063012	1
fischar gmbh	Glycerol 85%	5063012	1
Fischar/Anzag	Glycerol 85%	5063012	1
LAMOTTE/NOWEDA	Glycerol 85%	5538401	4
hedinger/anzag	Glycerol 85%	5538401	1
Lamotte/Noweda	Glycerol 85%	5538401	1
Gehe	Glycerol 85%	test1	1
Bombastus	Glycerol 85%	269070	2
Bombastus	Glycerol 85%	271511	2
Bombastus	Glycerol 85%	266037	1
Caelo	Glycerol 85%	213E-01589	1
Hedinger	Glycerol 85%	40452	1
Caelo	Glycerol 85%	3121202	1
Hedinger	Glycerol 85%	40447	1
Hedinger/Holdermann 18...	Glycerol 85%	40452	1
Gehe	Glycerol 85%	272305	1
Gehe	Glycerol 85%	40455	1
Hedinger / Sanacorp	Glycerol 85%	40451	1
Noweda	Glycerol 85%	40464	1
Phönix 06.10.2012	Glycerol 85%	40467	1
Phönix/Hedinger	Glycerol 85%	40471	1
Hedinger/Anzag 20.12.2...	Glycerol 85%	40467	2
Sanacorp/ Heddinger	Glycerol 85%	4071	2
Gehe	Glycerol 85%	1001017-01	1
Euro OTC	Glycerol 85%	1108032-01	5
Noweda	Glycerol 85%	40473	1
Euro OTC	Glycerol 85%	1108032	1
Caelo	Glycerol 85%	1121303	1
Caelo	Glycerol 85%	11324204	1
Caelo	Glycerol 85%	112117302	1
Fagron	Glycerol 85%	1203C003	1
Anzag	Glycerol 85%	120103801	1
Caelo	Glycerol 85%	12069603	2
Caelo	Glycerol 85%	12108202	1
Fagron	Glycerol 85%	12H16-N04	3
Euro OTC	Glycerol 85%	12o1038-01	1
Alliance Healthcare	Glycerol 85%	13144605	1

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Supplier	Substance	Batch	Spectra
Phönix	Glycerol 85%	13039203	1
Caelo	Glycerol 85%	20061210	1
Caelo	Glycerol 85%	19021301	1
Henry Lamotte	Glycerol 85%		1
Caelo	Glycerol 85%	20211212-2	1
Phönix Gotha	Glycerol 85%	275075	1
Hedinger Phönix	Glycerol 85%	40475	1
Bombastus	Glycerol 85%	275076	1
Gehe/Fischer	Glycerol 85%	5060061	1
Fischer otto,Saarbrücken	Glycerol 85%	5060091	1
Fischar	Glycerol 85%	5061101	1
Otto Fischar	Glycerol 85%	5062011	2
Otto Fischer GmbH Saarb...	Glycerol 85%	5061011	1
Fischar	Glycerol 85%	5062051	3
Fischar/Phönix	Glycerol 85%	5062051	1
Otto Fischar	Glycerol 85%	5062051	1
Caelo	Glycerol 85%	5062111	1
Gehe	Glycerol 85%	5226901	1
Noweda	Glycerol 85%	5226901	1
Lamotte	Glycerol 85%	5142501	1
Phönix/Lamotte	Glycerol 85%	5226901	5
Fagron	Glycerol 85%	Ch12L04-N09	1
Caesar & Loretz GmbH	Glycerol 85%	12216603	1
Fagron	Glycerol 85%	12L04-N09	1
Sanacorp	Glycerol 85%	13039204	1
Caesar & Loretz GmbH	Glycerol 85%	13144606	1
Ahd/PharmachemPößneck	Glycerol 85%	13248201	1
Fagron	Glycerol 85%	14A10-B01-291982	1
Fagron	Glycerol 85%	14D25-B02-295895	1
Otto Fischar	Glycerol 85%	5060121	1
Fischar	Glycerol 85%	5063051	1
Fischar	Glycerol 85%	5063052	1
Hedinger Phönix	Glycerol 85%	40542	1
Hedinger Gehe	Glycerol 85%	40519	1
Hedinger Phönix	Glycerol 85%	40548	1
Caelo	Glycerol 85%	1601059-01	1
Caelo	Glycerol 85%	16215303	1
Bombastus	Glycerol 85%	300395	2
Fischar/AHD	Glycerol 85%	5065031	1
Gehe	Glycerol 85%	11355301	1
Anzag	Glycerol 85%	40471	1
Anzag	Glycerol 85%	40467	1
Gehe	Glycerol 85%	276850	2
Gehe	Glycerol 85%	284401	1

- 57 058 spectra from 332 *Apo-Ident* customers from a total of 19 718 batches from a further 328 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 *Glycerol 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 *Glycerol 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	390	0	33 954
Type B	0	470	0	63 033
Type C	0	1359	24	57 058

The substance/substance group *Glycerol 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 % (> 99.9689 %)	100.0000 % (> 98.4615 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 98.7234 %)
Type C	100.0000 % (> 99.5963 %)	98.2646 % (> 98.0477 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30886	31737	2.56	60.45
30980	31956	1.70	61.88
31360	31956	1.68	61.04
31377	31737	1.16	63.21
31588	31588	0.00	60.93
31719	31719	0.00	63.06
31737	31737	0.00	63.77
31956	31956	0.00	62.84

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Glycolic acid 70%
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30491-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glycolic acid 70%; Acidum glycolicum 70%

Special notes

When selecting the *Glycolic acid 70%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Glycolic acid 70%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Glycolic acid 70%	1406006-01	31620	40	20140708
Euro OTC	Glycolic acid 70%	1406006-01	31647	40	20140708
Euro OTC	Glycolic acid 70%	1604050	32281	40	20160510*

Validation samples

A total of 156 379 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 *Glycolic acid 70%*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 4 reference samples from the substance/substance group *Glycolic acid 70%*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Glycolic acid 70%	1201002-01	30491	40
Euro OTC	Glycolic acid 70%	1406006-01	31620 [†]	20
Euro OTC	Glycolic acid 70%	1406006-01	31647 [†]	20
Euro OTC	Glycolic acid 70%	1604050-01	33225	40

- 63 474 spectra from a total of 1474 batches from further 439 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 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Glycolic acid 70%*.

*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.

[†]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*.

Supplier	Substance	Batch	Spectra
Euro OTC	Glycolic acid 70%	1109027-01	1
Caelo	Glycolic acid 70%	121002201	2
Euro OTC	Glycolic acid 70%	1210022-01	1
Phoenix	Glycolic acid 70%	1205037-01	1

- 58 436 spectra from 332 *Apo-Ident* customers from a total of 20 088 batches from a further 328 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 *Glycolic acid 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 *Glycolic acid 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	120	0	34 224
Type B	0	120	0	63 474
Type C	0	5	0	58 436

The substance/substance group *Glycolic acid 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.5981 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31620	32281	1.56	129.88
31647	32281	3.86	130.01
32281	32281	0.00	130.33

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Guaiazulene 25%, water-soluble**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30857-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Guaiazulene 25%, water-soluble

Special notes

When selecting the *Guaiazulene 25%, water-soluble* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Guaiazulene 25%, water-soluble*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Guaiazulene 25%,...	12246703	30857	40	20120831
Caelo	Guaiazulene 25%,...	13334401	31157	40	1411565
Caelo	Guaiazulene 25%,...	14130601	31462	40	20140423

Validation samples

A total of 156 379 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 *Guaiazulene 25%, water-soluble*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Guaiazulene 25%, water-soluble*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Guaiazulene 25%, water-soluble	14130601	31462 [†]	20
Caelo	Guaiazulene 25%, water-soluble	161905	32321	40

- 63 534 spectra from a total of 1475 batches from further 439 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.

- 91 spectra from 48 *Apo-Ident* customers from 34 batches from the substance/substance group *Guaiazulene 25%, water-soluble*.

Supplier	Substance	Batch	Spectra
Phönix	Guaiazulene 25%, water-soluble	12G31-N03	1
Caelo	Guaiazulene 25%, water-soluble	13044906	4

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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*.

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Guaiazulene 25%, water-soluble	4/AKD2	1
Euro OTC	Guaiazulene 25%, water-soluble	13334406	1
Caelo	Guaiazulene 25%, water-soluble	516Q-03150	1
Caelo	Guaiazulene 25%, water-soluble	14130601	3
Caelo	Guaiazulene 25%, water-soluble	13334407	3
Caelo	Guaiazulene 25%, water-soluble	14130605	1
Caelo	Guaiazulene 25%, water-soluble	14252102	4
Caelo	Guaiazulene 25%, water-soluble	14252104	3
Fagron	Guaiazulene 25%, water-soluble	14B12-B07-292053	1
Fagron	Guaiazulene 25%, water-soluble	14C24-B03-29675	1
Caelo	Guaiazulene 25%, water-soluble	15075501	4
Caelo	Guaiazulene 25%, water-soluble	15075503	3
Fagron	Guaiazulene 25%, water-soluble	152716-0001	1
Caelo	Guaiazulene 25%, water-soluble	15402306	1
Caelo	Guaiazulene 25%, water-soluble	1515M-03150	1
Caelo	Guaiazulene 25%, water-soluble	15402302	1
Caesar & Loretz GmbH Hi...	Guaiazulene 25%, water-soluble	15402306	1
Caelo	Guaiazulene 25%, water-soluble	17041405	1
Fagron	Guaiazulene 25%, water-soluble	11H30-N03	1
Caelo	Guaiazulene 25%, water-soluble	13334406	3
Caelo	Guaiazulene 25%, water-soluble	11303702	2
Caelo	Guaiazulene 25%, water-soluble	1514U-03150	1
Caelo	Guaiazulene 25%, water-soluble	13044901	9
Caelo	Guaiazulene 25%, water-soluble	11303703	1
Caelo	Guaiazulene 25%, water-soluble	12158701	2
Post-Apotheke	Guaiazulene 25%, water-soluble	12246701	1
Caelo	Guaiazulene 25%, water-soluble	12019802	1
Caelo	Guaiazulene 25%, water-soluble	12246701	3
Caelo	Guaiazulene 25%, water-soluble	12246703	3
Caelo	Guaiazulene 25%, water-soluble	12246704	4
Fagron	Guaiazulene 25%, water-soluble	12G31-N03	1
Noweda	Guaiazulene 25%, water-soluble	12G31-N03	1
Alliance Healthcare	Guaiazulene 25%, water-soluble	13044901	1
Caelo	Guaiazulene 25%, water-soluble	13044904	8
Noweda	Guaiazulene 25%, water-soluble	13044901	1
Caelo	Guaiazulene 25%, water-soluble	13334401	5
Großhandel	Guaiazulene 25%, water-soluble	13334401	1
Caelo	Guaiazulene 25%, water-soluble		1
Fagron	Guaiazulene 25%, water-soluble	13g31-n03	1
Gehe	Guaiazulene 25%, water-soluble	13334406	1
Fagron	Guaiazulene 25%, water-soluble	513936	1
Sanacorp	Guaiazulene 25%, water-soluble	12246701	1

- 58 350 spectra from 332 *Apo-Ident* customers from a total of 20 060 batches from a further 328 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 *Guaiazulene 25%, water-soluble* 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 *Guaiazulene 25%, water-soluble* 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	34 224
Type B	0	60	0	63 534
Type C	0	78	13	58 350

The substance/substance group *Guaiazulene 25%, water-soluble* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.5964 %)	85.7143 % (> 82.4176 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30857	31157	2.72	60.99
31157	31157	0.00	61.71
31462	31157	4.03	63.53

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Hard fat 649**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30770-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Hard fat 649; Adeps solidus 649

Special notes

When selecting the *Hard fat 649* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Hard fat 649*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Hard fat 649	12I10-N12	30770	40	1407601
Fagron	Hard fat 649	15E13-B01-307859	31699	40	20150527

Validation samples

A total of 156 379 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 *Hard fat 649*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Hard fat 649*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Hard fat 649	13C19-N03	31118	40
Fagron	Hard fat 649	15E13-B01-307859	31699 [†]	20

- 63 534 spectra from a total of 1475 batches from further 439 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 *Hard fat 649*.

Supplier	Substance	Batch	Spectra
Fagron	Hard fat 649	105945	1

[†]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*.

- 58 440 spectra from 332 *Apo-Ident* customers from a total of 20 091 batches from a further 328 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 *Hard fat 649* 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 *Hard fat 649* 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	34 264
Type B	0	59	1	63 534
Type C	0	1	0	58 440

The substance/substance group *Hard fat 649* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	98.3333 % (> 93.3333 %)
Type C	100.0000 % (> 99.6053 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30770	30770	0.00	26.35
31699	30770	10.69	21.86

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Honeys**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30548-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Honeys; Honey; Mel; Mel rosatum; Rose honey

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Honeys*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Rose honey	12105302	30548	40	1403099
Caelo	Honey	12132005	30761	40	1402562
Caelo	Honey	13269412	31341	40	20130913
Caelo	Rose honey	15406006	31957	40	20160120

Validation samples

A total of 156 379 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 *Honeys*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 794 batches from further 223 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 180 spectra of 5 reference samples from the substance/substance group *Honeys*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Honey	11187911	30610	40
Caelo	Rose honey	15406006	31957 [†]	20
Caelo	Honey	150791	32214	40
Caelo	Honey	162659	32698	40
Caelo	Rose honey	16104802	32988	40

- 63 414 spectra from a total of 1472 batches from further 438 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.

- 48 spectra from 16 *Apo-Ident* customers from 31 batches from the substance/substance group *Honeys*.

[†]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*.

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH, 4...	Honey	12132011	2
Caelo	Honey	12382406	1
Caesar & Loretz GmbH, 4...	Honey	12382405	4
Caelo	Honey	13269413	1
Caelo	Honey	13269412	3
Caesar & Loretz GmbH, 4...	Honey	13269404	1
Euro OTC	Honey	13269401	3
Caelo	Honey	12132012	1
Caelo	Honey	12132007	1
Caesar & Loretz GmbH, 4...	Honey	12382410	2
Noweda/Apomix	Honey	13269401	1
Caelo	Honey	13269403	3
Caelo	Honey	13269405	2
Phönix	Honey	13269403	1
Caelo	Honey	15079103	1
Caelo	Honey	15079111	1
Caelo	Rose honey	14125607	1
Caelo	Rose honey	5091401	1
Caelo	Rose honey	11258901	1
Caelo	Rose honey	12105305	2
Caelo	Rose honey	12315003	1
Caelo	Rose honey	12105302	1
Caelo	Rose honey	12315005	2
Caelo	Rose honey	13170902	1
Caelo	Rose honey	13170906	1
Caelo	Rose honey	13170904	1
Caelo	Rose honey	14125603	1
Caelo	Rose honey	14125605	1
Caelo	Rose honey	15100801	2
Caelo	Rose honey	4811M-02884	1
Caelo	Rose honey	15406004	1
Caelo	Rose honey	15100803	1
Ebert & Jacobi 02.08.16	Rose honey	15406006	1

- 58 393 spectra from 332 *Apo-Ident* customers from a total of 20 061 batches from a further 327 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 *Honeys* 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 *Honeys* 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	34 184
Type B	0	179	1	63 414
Type C	0	48	0	58 393

The substance/substance group *Honeys* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	99.4444 % (> 97.7778 %)
Type C	100.0000 % (> 99.5965 %)	100.0000 % (> 87.5000 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30548	30548	0.00	26.48
30761	30761	0.00	35.56
31341	30761	6.86	20.63
31957	30548	9.16	29.39

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Hydrophilic base emulsion (NRF p.25)
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30709-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydrophilic base emulsion (NRF p.25); Emulsio basalis hydrophilica

Special notes

When selecting the *Hydrophilic base emulsion (NRF p.25)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 base emulsion (NRF p.25)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydrophilic base...	12173002	30709	30	20120628
Caelo	Hydrophilic base...	13305501	31176	40	1403535
Caelo	Hydrophilic base...	14063502	31340	20	20140307
Caelo	Hydrophilic base...	161155	32291	40	20160415*
Caelo	Hydrophilic base...	170444	33154	40	20170217*

Validation samples

A total of 156379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 170 spectra of 5 reference samples from the substance/substance group *Hydrophilic base emulsion* (NRF p.25). These samples are listed above in the [calibration samples](#) section.
- 34174 spectra from a total of 793 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 151 spectra of 5 reference samples from the substance/substance group *Hydrophilic base emulsion* (NRF p.25).

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrophilic base emulsion (N...	11129901	30334	41
Caelo	Hydrophilic base emulsion (N...	12173002	30709 [†]	10
Caelo	Hydrophilic base emulsion (N...	14063502	31340 [†]	20
Caelo	Hydrophilic base emulsion (N...	161156	32290	40
Caelo	Hydrophilic base emulsion (N...	161154	32292	40

- 63443 spectra from a total of 1472 batches from further 439 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.

- 763 spectra from 143 *Apo-Ident* customers from 142 batches from the substance/substance group *Hydrophilic base emulsion* (NRF p.25).

*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.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Hydrophilic base emulsion (N...	13394302	11
Caelo	Hydrophilic base emulsion (N...	13394304	6
Caelo	Hydrophilic base emulsion (N...	14063502	13
Caelo	Hydrophilic base emulsion (N...	13397601	40
Caelo	Hydrophilic base emulsion (N...	14063601	20
Sanacorp	Hydrophilic base emulsion (N...	14063601	3
Caelo	Hydrophilic base emulsion (N...	14063702	4
Caelo	Hydrophilic base emulsion (N...	14238901	23
Caelo	Hydrophilic base emulsion (N...	14238801	14
Sanacorp	Hydrophilic base emulsion (N...	14141004	1
Caelo	Hydrophilic base emulsion (N...	14140901	6
Caelo	Hydrophilic base emulsion (N...	14238101	1
Caelo	Hydrophilic base emulsion (N...	14360201	8
Caelo	Hydrophilic base emulsion (N...	14351202	4
Caelo	Hydrophilic base emulsion (N...	1515J-03325	1
Caelo	Hydrophilic base emulsion (N...	14360301	26
Caelo	Hydrophilic base emulsion (N...	15209801	17
Caelo	Hydrophilic base emulsion (N...	15440001	5
Caelo	Hydrophilic base emulsion (N...	23011503	1
Caelo	Hydrophilic base emulsion (N...	13039701	9
Caelo	Hydrophilic base emulsion (N...	12310101	12
Caelo	Hydrophilic base emulsion (N...	13076702	11
Caelo	Hydrophilic base emulsion (N...	12173002	5
Caelo	Hydrophilic base emulsion (N...	15440101	14
Caelo	Hydrophilic base emulsion (N...	13076801	13
Caelo	Hydrophilic base emulsion (N...	12128401	5
Phönix	Hydrophilic base emulsion (N...	13039701	1
Phönix	Hydrophilic base emulsion (N...	13076803	1
Caelo	Hydrophilic base emulsion (N...	13107703	14
Caelo	Hydrophilic base emulsion (N...	13076803	21
Caelo	Hydrophilic base emulsion (N...	13195801	11
Caelo	Hydrophilic base emulsion (N...	13196001	6
Caelo	Hydrophilic base emulsion (N...	13305401	21
Caelo	Hydrophilic base emulsion (N...	13305601	11
Caelo	Hydrophilic base emulsion (N...	13305501	8
aliance healthcare 5.12...	Hydrophilic base emulsion (N...	13305501	1
Henry Lamotte Oils Gmbh...	Hydrophilic base emulsion (N...	13397601	2
Caesar&loretz,AHC	Hydrophilic base emulsion (N...	14063601	1
Caelo	Hydrophilic base emulsion (N...	30011504	1
Caelo	Hydrophilic base emulsion (N...	28111203	1
Caelo	Hydrophilic base emulsion (N...	30041304	1
Caelo	Hydrophilic base emulsion (N...	914E-03325	1
Caesar & Lorenz	Hydrophilic base emulsion (N...	14238901	1
Caelo	Hydrophilic base emulsion (N...	15337601	2
Caelo	Hydrophilic base emulsion (N...	1514U-03325	1
Caeo/Noweda	Hydrophilic base emulsion (N...	15440001	1
Caelo	Hydrophilic base emulsion (N...	16115602	11
Caelo	Hydrophilic base emulsion (N...	16249201	3
Caelo	Hydrophilic base emulsion (N...	12230203	6
Caelo	Hydrophilic base emulsion (N...	16249301	2
Caelo	Hydrophilic base emulsion (N...	16264101	5
Caelo	Hydrophilic base emulsion (N...	12310102	13
Caelo	Hydrophilic base emulsion (N...	12288103	2
Caelo	Hydrophilic base emulsion (N...	13039702	1
Caelo	Hydrophilic base emulsion (N...	13195901	15
Caesar & Lorenz	Hydrophilic base emulsion (N...	13195901	1
Caelo	Hydrophilic base emulsion (N...	1071602	1
Caelo	Hydrophilic base emulsion (N...	2061501	1
Caelo	Hydrophilic base emulsion (N...	11031504	1
Gehe am 6.03.2014	Hydrophilic base emulsion (N...	13195801	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrophilic base emulsion (N...	13305503	4
Caelo	Hydrophilic base emulsion (N...	13394032	1
GEHE 2.04.2014	Hydrophilic base emulsion (N...	13394302	2
Phoenix	Hydrophilic base emulsion (N...	13394304	2
Caelo	Hydrophilic base emulsion (N...	13394402	2
gehe	Hydrophilic base emulsion (N...	13394402	2
Caesar&Loretz GmbH/Anzag	Hydrophilic base emulsion (N...	13397601	1
Caelo	Hydrophilic base emulsion (N...	13730153	1
GEHE 14.04.2014	Hydrophilic base emulsion (N...	14063502	2
AHD	Hydrophilic base emulsion (N...	14063502	2
gehe	Hydrophilic base emulsion (N...	14063503	1
PHOENIX 03.06.2014	Hydrophilic base emulsion (N...	14063701	1
Gehe	Hydrophilic base emulsion (N...	14063702	1
Gehe	Hydrophilic base emulsion (N...	1410901	1
Gehe	Hydrophilic base emulsion (N...	14140901	1
Caelo	Hydrophilic base emulsion (N...	14141003	2
Caelo	Hydrophilic base emulsion (N...	14141004	9
Caelo	Hydrophilic base emulsion (N...	14238701	11
Caelo	Hydrophilic base emulsion (N...	14238702	4
Gehe	Hydrophilic base emulsion (N...	14238702	1
Caelo	Hydrophilic base emulsion (N...	14238802	3
Gehe	Hydrophilic base emulsion (N...	14238802	1
Sanacorp	Hydrophilic base emulsion (N...	14238901	1
Caelo	Hydrophilic base emulsion (N...	14239103	3
Caelo	Hydrophilic base emulsion (N...	1428901	1
Alliance health	Hydrophilic base emulsion (N...	14360201	2
Caelo	Hydrophilic base emulsion (N...	14360202	2
Sanacorp	Hydrophilic base emulsion (N...	14360301	1
Caelo	Hydrophilic base emulsion (N...	14360401	2
Caelo	Hydrophilic base emulsion (N...	14360403	2
Caelo	Hydrophilic base emulsion (N...	1463502	1
Caelo	Hydrophilic base emulsion (N...	15029901	1
Caelo	Hydrophilic base emulsion (N...	15076803	4
Caelo	Hydrophilic base emulsion (N...	15076901	7
Caelo	Hydrophilic base emulsion (N...	15077002	8
Caelo	Hydrophilic base emulsion (N...	15077003	4
Caelo	Hydrophilic base emulsion (N...	15077101	14
Caelo	Hydrophilic base emulsion (N...	15077101	3
Caesar&Loretz GmbH/Anzag	Hydrophilic base emulsion (N...	15077101	2
Caelo	Hydrophilic base emulsion (N...	15081402	1
Noweda	Hydrophilic base emulsion (N...	15209801	1
Caelo	Hydrophilic base emulsion (N...	15209901	2
cealo/noveda	Hydrophilic base emulsion (N...	15209901	1
Caelo	Hydrophilic base emulsion (N...	15209902	3
Caelo	Hydrophilic base emulsion (N...	15210001	6
Sanacorp	Hydrophilic base emulsion (N...	15337301	2
Caelo	Hydrophilic base emulsion (N...	15337301	13
Caesar&Loretz GmbH	Hydrophilic base emulsion (N...	15337301	1
Eigen/Defektur	Hydrophilic base emulsion (N...	15337602	1
Caelo	Hydrophilic base emulsion (N...	15337701	4
Caelo	Hydrophilic base emulsion (N...	15337801	10
Caelo	Hydrophilic base emulsion (N...	15439801	8
Caesar & Loretz GmbH Hi...	Hydrophilic base emulsion (N...	15439801	1
Caesar&Loretz GmbH/ Gehe	Hydrophilic base emulsion (N...	15439801	1
Caesar&Loretz GmbH	Hydrophilic base emulsion (N...	15439801	1
Caelo	Hydrophilic base emulsion (N...	15439901	3
Caelo	Hydrophilic base emulsion (N...	15440002	2
Caelo	Hydrophilic base emulsion (N...	15440102	1
Caelo	Hydrophilic base emulsion (N...	154401014	1
Caelo	Hydrophilic base emulsion (N...	16115302	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrophilic base emulsion (N...	16115303	5
Caelo	Hydrophilic base emulsion (N...	16115401	2
Caesar & Loretz GmbH Hi...	Hydrophilic base emulsion (N...	16115602	1
Ebert 12.09.2016	Hydrophilic base emulsion (N...	16115602	1
Caesar & Loretz GmbH Hi...	Hydrophilic base emulsion (N...	16151602	1
Caelo	Hydrophilic base emulsion (N...	16264202	1
Caesar&Loretz GmbH/ All...	Hydrophilic base emulsion (N...	16264202	1
Caelo	Hydrophilic base emulsion (N...		1
Caelo	Hydrophilic base emulsion (N...	18081512	1
Caelo	Hydrophilic base emulsion (N...	20061407	1
Caelo	Hydrophilic base emulsion (N...	21031403	1
Caelo	Hydrophilic base emulsion (N...	23071507	1
Caelo	Hydrophilic base emulsion (N...	29041406	1
Caelo	Hydrophilic base emulsion (N...	29041502	1
Caelo	Hydrophilic base emulsion (N...	29101402	1
Caelo	Hydrophilic base emulsion (N...	30051501	1
Caelo	Hydrophilic base emulsion (N...	2101304	1
Maros	Hydrophilic base emulsion (N...	5006613	1
Caelo	Hydrophilic base emulsion (N...	6138389	1
Caelo	Hydrophilic base emulsion (N...	6051304	1
Caelo	Hydrophilic base emulsion (N...	9081301	1
Caelo	Hydrophilic base emulsion (N...	10071203	1
Caelo	Hydrophilic base emulsion (N...	10051303	1
Caelo	Hydrophilic base emulsion (N...	11274003	1
Gehe	Hydrophilic base emulsion (N...	12047602	4
Noweda	Hydrophilic base emulsion (N...	12071901	1
Anzag ek:4,35EUR	Hydrophilic base emulsion (N...	12071901	2
Caelo	Hydrophilic base emulsion (N...	12071901	2
Caesar/Noweda	Hydrophilic base emulsion (N...	12071901	1
Caelo	Hydrophilic base emulsion (N...	12072002	2
Gehe	Hydrophilic base emulsion (N...	12072002	1
Caelo	Hydrophilic base emulsion (N...	12121308	1
Gehe	Hydrophilic base emulsion (N...	12128401	1
Fiebig ek:4,26EUR 18.09.12	Hydrophilic base emulsion (N...	12173003	1
Caelo	Hydrophilic base emulsion (N...	1213003	1
Caelo	Hydrophilic base emulsion (N...	1218401	1
Caelo	Hydrophilic base emulsion (N...	12173003	1
Caelo	Hydrophilic base emulsion (N...	12230301	8
Noweda	Hydrophilic base emulsion (N...	12230301	2
Anzag 27.11.12 ek:4,33	Hydrophilic base emulsion (N...	12230301	1
Caelo	Hydrophilic base emulsion (N...	12230302	5
Gehe am 07.03.2013	Hydrophilic base emulsion (N...	12310101	1
Caesar & Loretz GmbH, 4...	Hydrophilic base emulsion (N...	12310101	1
Anzag 11.01.13	Hydrophilic base emulsion (N...	12310102	3
Noweda	Hydrophilic base emulsion (N...	12310102	1
Phoenix 11.03.13	Hydrophilic base emulsion (N...	13039701	2
A.H. 23.05.13 ek:4,56	Hydrophilic base emulsion (N...	13039701	4
Caelo	Hydrophilic base emulsion (N...	1306801	1
Noweda	Hydrophilic base emulsion (N...	13076801	1
Caelo	Hydrophilic base emulsion (N...	13076802	1
Gehe 29.04.2013	Hydrophilic base emulsion (N...	13076803	2
Celo	Hydrophilic base emulsion (N...	1307681	1
Caelo	Hydrophilic base emulsion (N...	13107702	1
Gehe	Hydrophilic base emulsion (N...	13195801	1
AHC 15.08.13 EK4,56	Hydrophilic base emulsion (N...	13107703	1
Caelo	Hydrophilic base emulsion (N...	1310773	2
Caesar & Loretz GmbH, 4...	Hydrophilic base emulsion (N...	13107703	1
Phönix Gotha	Hydrophilic base emulsion (N...	13195801	1
Phönix	Hydrophilic base emulsion (N...	13195801	1
Caesar & Loretz	Hydrophilic base emulsion (N...	13195801	1

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Supplier	Substance	Batch	Spectra
Caesar&Loretz GmbH/Anzag	Hydrophilic base emulsion (N...	13195901	1
Sanacorp	Hydrophilic base emulsion (N...	13195901	1
Fagron	Hydrophilic base emulsion (N...	13195901	1
Caelo	Hydrophilic base emulsion (N...	13195902	1
gehe	Hydrophilic base emulsion (N...	13196001	1
Sanacorp	Hydrophilic base emulsion (N...	13305401	5
Fagron	Hydrophilic base emulsion (N...	13305401	5
gehe	Hydrophilic base emulsion (N...	13305401	1
PHOENIX am 27.01.2014	Hydrophilic base emulsion (N...	13305401	1
Caelo	Hydrophilic base emulsion (N...	13394303	1
Sanacorp	Hydrophilic base emulsion (N...	13397601	2
Phoenix	Hydrophilic base emulsion (N...	14063502	1
Phonix	Hydrophilic base emulsion (N...	14063601	1
Caelo	Hydrophilic base emulsion (N...	20031306	1
Phoenix	Hydrophilic base emulsion (N...	14063701	1
Caelo	Hydrophilic base emulsion (N...	26031302	1
Caelo	Hydrophilic base emulsion (N...	24011403	1
Caelo	Hydrophilic base emulsion (N...	23101202	1
Caelo	Hydrophilic base emulsion (N...	28121206	1
Caesar/Noweda	Hydrophilic base emulsion (N...	5011E-03325	1
Caelo	Hydrophilic base emulsion (N...	26031305	1
Caelo	Hydrophilic base emulsion (N...	26031303	1
Sanacorp	Hydrophilic base emulsion (N...		1
Gehe	Hydrophilic base emulsion (N...	11223501	2
Gehe	Hydrophilic base emulsion (N...	11274003	1
Gehe	Hydrophilic base emulsion (N...	11273902	1
Noweda	Hydrophilic base emulsion (N...	12173003	1
Kehr	Hydrophilic base emulsion (N...	12047601	1
Gehe	Hydrophilic base emulsion (N...	12071902	2
Gehe	Hydrophilic base emulsion (N...	12230203	2
Caelo	Hydrophilic base emulsion (N...	1223030	1
Gehe	Hydrophilic base emulsion (N...	13076702	1
Phoenix	Hydrophilic base emulsion (N...	13195901	1
Herstellung	Hydrophilic base emulsion (N...	13305501	2
Phoenix	Hydrophilic base emulsion (N...	13397601	1
Caelo	Hydrophilic base emulsion (N...	16071701	1
Caelo	Hydrophilic base emulsion (N...	15061302	1
Caelo	Hydrophilic base emulsion (N...	19091204	1
Caelo	Hydrophilic base emulsion (N...	18111307	1

- 57 678 spectra from 332 *Apo-Ident* customers from a total of 19 955 batches from a further 328 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 base emulsion (NRF p.25)* 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 base emulsion (NRF p.25)* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	170	0	34 174
Type B	0	138	13	63 397
Type C	0	739	24	57 674

The substance/substance group *Hydrophilic base emulsion (NRF p.25)* 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 % (> 99.9690 %)	100.0000 % (> 96.4706 %)
Type B	100.0000 % (> 99.9711 %)	91.3907 % (> 89.4040 %)
Type C	100.0000 % (> 99.5978 %)	96.8545 % (> 96.4613 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30709	32291	3.76	22.16
31176	31176	0.00	28.61
31340	33154	8.03	26.90
32291	32291	0.00	26.15
33154	33154	0.00	30.58

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Hydrophilic cream, non-ionic DAB
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30463-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydrophilic cream, non-ionic DAB; Unguentum emulsificans nonionicum aquosum DAB

Special notes

When selecting the *Hydrophilic cream, non-ionic DAB* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 cream, non-ionic DAB*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydrophilic crea...	13138001	31001	40	20130531
Caelo	Hydrophilic crea...	13332901	31227	40	20131104
Caelo	Hydrophilic crea...	13333101	31451	40	1509156
Caelo	Hydrophilic crea...	15151601	31748	40	9129
Bombastus	Hydrophilic crea...	295368	31749	30	20150625
Caelo	Hydrophilic crea...	161042	32088	40	20160411*
Bombastus	Hydrophilic crea...	300481	32105	40	20160225
Bombastus	Hydrophilic crea...	300481	32726	40	20160225

Validation samples

A total of 156379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 310 spectra of 8 reference samples from the substance/substance group *Hydrophilic cream, non-ionic DAB*. These samples are listed above in the [calibration samples](#) section.
- 34034 spectra from a total of 791 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 960 spectra of 25 reference samples from the substance/substance group *Hydrophilic cream, non-ionic DAB*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrophilic cream, non-ionic...	11273301	30463	40
Caelo	Hydrophilic cream, non-ionic...	15151601	31748 [†]	20
Bombastus	Hydrophilic cream, non-ionic...	295368	31749 [†]	30
Caelo	Hydrophilic cream, non-ionic...	153446	32077	40
Caelo	Hydrophilic cream, non-ionic...	153447	32078	40
Caelo	Hydrophilic cream, non-ionic...	153463	32084	40
Caelo	Hydrophilic cream, non-ionic...	161045	32085	40
Caelo	Hydrophilic cream, non-ionic...	161041	32087	40
Caelo	Hydrophilic cream, non-ionic...	153465	32106	40
Caelo	Hydrophilic cream, non-ionic...	160438	32107	40
Caelo	Hydrophilic cream, non-ionic...	161041	32108	40
Caelo	Hydrophilic cream, non-ionic...	161042	32109	30
Caelo	Hydrophilic cream, non-ionic...	161043	32110	40
Caelo	Hydrophilic cream, non-ionic...	161043	32111	40
Caelo	Hydrophilic cream, non-ionic...	161044	32112	40
Caelo	Hydrophilic cream, non-ionic...	161044	32113	40
Caelo	Hydrophilic cream, non-ionic...	161045	32114	40
Caelo	Hydrophilic cream, non-ionic...	161735	32417	40
Caelo	Hydrophilic cream, non-ionic...	161736	32418	40
Caelo	Hydrophilic cream, non-ionic...	161793	32419	40
Caelo	Hydrophilic cream, non-ionic...	161793	32420	40
Caelo	Hydrophilic cream, non-ionic...	161794	32421	40

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

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrophilic cream, non-ionic...	162348	32488	40
Caelo	Hydrophilic cream, non-ionic...	162349	32489	40
Caelo	Hydrophilic cream, non-ionic...	162350	32490	40

- 62 634 spectra from a total of 1457 batches from further 439 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.

- 372 spectra from 124 *Apo-Ident* customers from 128 batches from the substance/substance group *Hydrophilic cream, non-ionic DAB*.

Supplier	Substance	Batch	Spectra
Caelo	Hydrophilic cream, non-ionic...	13333101	9
Caelo	Hydrophilic cream, non-ionic...	13332901	7
Caelo	Hydrophilic cream, non-ionic...	13333201	2
Caelo	Hydrophilic cream, non-ionic...	14068601	11
Caelo	Hydrophilic cream, non-ionic...	14068801	2
Caelo	Hydrophilic cream, non-ionic...	14259001	5
Caelo	Hydrophilic cream, non-ionic...	15002901	9
Caelo	Hydrophilic cream, non-ionic...	15007402	4
Noweda08.06.2015	Hydrophilic cream, non-ionic...	15027801	1
Caelo	Hydrophilic cream, non-ionic...	15027801	14
Caelo	Hydrophilic cream, non-ionic...	15105001	2
Caelo	Hydrophilic cream, non-ionic...	15105101	7
Caelo	Hydrophilic cream, non-ionic...	15105201	1
Caelo	Hydrophilic cream, non-ionic...	15151801	2
Caelo	Hydrophilic cream, non-ionic...	15286701	3
Caelo	Hydrophilic cream, non-ionic...	15287001	9
Caelo	Hydrophilic cream, non-ionic...	15346401	2
Phoenix	Hydrophilic cream, non-ionic...	16104501	2
Caelo	Hydrophilic cream, non-ionic...	16104101	8
Bombastus	Hydrophilic cream, non-ionic...	282902	1
Bombastus	Hydrophilic cream, non-ionic...	293401	1
Bombastus	Hydrophilic cream, non-ionic...	300481	3
Caelo	Hydrophilic cream, non-ionic...	300481	2
Bombastus	Hydrophilic cream, non-ionic...	271981	3
Bombastus	Hydrophilic cream, non-ionic...	272063	3
Caelo	Hydrophilic cream, non-ionic...	11357601	2
Caelo	Hydrophilic cream, non-ionic...	11357502	1
Caelo	Hydrophilic cream, non-ionic...	12086901	3
Caelo	Hydrophilic cream, non-ionic...	12001602	1
Caelo	Hydrophilic cream, non-ionic...	12087001	4
Caelo	Hydrophilic cream, non-ionic...	12156101	2
Caelo	Hydrophilic cream, non-ionic...	12155801	2

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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
phönix 22.01.2013	Hydrophilic cream, non-ionic...	12156101	1
Fagron	Hydrophilic cream, non-ionic...	12223301	3
Caelo	Hydrophilic cream, non-ionic...	12223501	3
Caelo	Hydrophilic cream, non-ionic...	12352801	7
Caelo	Hydrophilic cream, non-ionic...	12353001	1
Fagron	Hydrophilic cream, non-ionic...	13045301	1
Caelo	Hydrophilic cream, non-ionic...	13045501	3
Caelo	Hydrophilic cream, non-ionic...	13138001	13
Caelo	Hydrophilic cream, non-ionic...	13045401	3
Caelo	Hydrophilic cream, non-ionic...	13138201	4
Caelo	Hydrophilic cream, non-ionic...	13138101	1
Caelo	Hydrophilic cream, non-ionic...	13263301	2
Caelo	Hydrophilic cream, non-ionic...	13263501	7
Caelo	Hydrophilic cream, non-ionic...	13138101	8
Caelo	Hydrophilic cream, non-ionic...	13333401	5
Noweda	Hydrophilic cream, non-ionic...	1812U-02543	1
Caelo	Hydrophilic cream, non-ionic...	21111203	1
Bombastus	Hydrophilic cream, non-ionic...	280909	3
Bombastus	Hydrophilic cream, non-ionic...	290283	3
Bombastus	Hydrophilic cream, non-ionic...	6861335	1
Berkel AHK	Hydrophilic cream, non-ionic...	13332901	3
GEHE 10.03.2014	Hydrophilic cream, non-ionic...	13137901	1
Caelo	Hydrophilic cream, non-ionic...	1333101	1
Caelo	Hydrophilic cream, non-ionic...	13263801	2
Caelo	Hydrophilic cream, non-ionic...	13333001	3
Berkel AHK	Hydrophilic cream, non-ionic...	13333101	2
Caelo	Hydrophilic cream, non-ionic...	13333301	3
Caelo	Hydrophilic cream, non-ionic...	13333501	5
Sanacorp	Hydrophilic cream, non-ionic...	14068601	1
Caelo	Hydrophilic cream, non-ionic...	14068401	1
Caelo	Hydrophilic cream, non-ionic...	14068701	2
Caelo	Hydrophilic cream, non-ionic...	14069001	5
Caelo	Hydrophilic cream, non-ionic...	14068901	1
Caelo	Hydrophilic cream, non-ionic...	14221301	1
GEHE 23.09.2014	Hydrophilic cream, non-ionic...	14221301	1
Caelo	Hydrophilic cream, non-ionic...	14221401	6
Caelo	Hydrophilic cream, non-ionic...	14221501	1
Caelo	Hydrophilic cream, non-ionic...	14258901	6
Caelo	Hydrophilic cream, non-ionic...	14259101	2
Caelo	Hydrophilic cream, non-ionic...	14259201	2
Sanacorp	Hydrophilic cream, non-ionic...	15002901	1
Caelo	Hydrophilic cream, non-ionic...	15002801	2
Caelo	Hydrophilic cream, non-ionic...	15027601	1
Caelo	Hydrophilic cream, non-ionic...	15151601	5
Caelo	Hydrophilic cream, non-ionic...	15286801	1
Caelo	Hydrophilic cream, non-ionic...	16043801	2
Caelo	Hydrophilic cream, non-ionic...	16104201	1
Gehe	Hydrophilic cream, non-ionic...	16104401	1
Caelo	Hydrophilic cream, non-ionic...	16173401	1
Caelo	Hydrophilic cream, non-ionic...	16173501	2
Caelo	Hydrophilic cream, non-ionic...	16179401	7
Caelo	Hydrophilic cream, non-ionic...	19081505	1
Caelo	Hydrophilic cream, non-ionic...	20061406	1
Bombastus	Hydrophilic cream, non-ionic...	286003	2
bom	Hydrophilic cream, non-ionic...	286003	1
Bombastus	Hydrophilic cream, non-ionic...	288043	3
Bombastus	Hydrophilic cream, non-ionic...	288044	2
Bombastus	Hydrophilic cream, non-ionic...	293403	2
Bombastus	Hydrophilic cream, non-ionic...	295368	1
Bombastus	Hydrophilic cream, non-ionic...	296803	2

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Supplier	Substance	Batch	Spectra
Caelo	Hydrophilic cream, non-ionic...	297634	1
Bombastus	Hydrophilic cream, non-ionic...	297634	1
Bombastus	Hydrophilic cream, non-ionic...	303642	1
Bombastus	Hydrophilic cream, non-ionic...	303640	1
Euro OTC	Hydrophilic cream, non-ionic...	266631	1
Bombastus	Hydrophilic cream, non-ionic...	258174	1
Bombastus	Hydrophilic cream, non-ionic...	267625	3
Bombastus	Hydrophilic cream, non-ionic...	271976	1
Bombastus	Hydrophilic cream, non-ionic...	271977	1
Noweda	Hydrophilic cream, non-ionic...	271980	2
Sanacorp	Hydrophilic cream, non-ionic...	271980	1
Bombasus, Noweda	Hydrophilic cream, non-ionic...	272063	1
Caelo	Hydrophilic cream, non-ionic...	513Q-02543	1
Caelo	Hydrophilic cream, non-ionic...	6061305	1
Caelo	Hydrophilic cream, non-ionic...	11273303	2
Caelo	Hydrophilic cream, non-ionic...	11273001	1
Caelo	Hydrophilic cream, non-ionic...	11273401	1
Caelo	Hydrophilic cream, non-ionic...	11357801	1
Caelo	Hydrophilic cream, non-ionic...	11357301	1
Caelo	Hydrophilic cream, non-ionic...	12086802	1
Caelo	Hydrophilic cream, non-ionic...	12086902	1
Caelo	Hydrophilic cream, non-ionic...	12155901	4
Phönix 25.09.2012	Hydrophilic cream, non-ionic...	12087001	1
Caelo	Hydrophilic cream, non-ionic...	12223301	1
Caelo	Hydrophilic cream, non-ionic...	12223602	1
Caelo	Hydrophilic cream, non-ionic...	12223601	2
Caesar &Loretz GmbH	Hydrophilic cream, non-ionic...	12352901	1
Caelo	Hydrophilic cream, non-ionic...	12352901	3
Caelo	Hydrophilic cream, non-ionic...	130450401	1
Caelo	Hydrophilic cream, non-ionic...	13045201	3
Sanacorp	Hydrophilic cream, non-ionic...	13045401	1
Caelo	Hydrophilic cream, non-ionic...	13045601	3
Hustadt Apotheke	Hydrophilic cream, non-ionic...	13045601	1
Caelo	Hydrophilic cream, non-ionic...	13137801	1
Caelo	Hydrophilic cream, non-ionic...	13137901	1
Martinus-Apotheke	Hydrophilic cream, non-ionic...	13138001	1
Noweda	Hydrophilic cream, non-ionic...	13138101	1
Post-Apotheke	Hydrophilic cream, non-ionic...	13138301	1
Caelo	Hydrophilic cream, non-ionic...	1318001	1
Caelo	Hydrophilic cream, non-ionic...	13263401	1
Caelo	Hydrophilic cream, non-ionic...	13263601	3
Caelo	Hydrophilic cream, non-ionic...	13263701	3
Post-Apotheke	Hydrophilic cream, non-ionic...	13263701	2
Caelo	Hydrophilic cream, non-ionic...	13263902	3
Caelo	Hydrophilic cream, non-ionic...	21081202	1
Bombastus	Hydrophilic cream, non-ionic...	275256	1
Bombastus	Hydrophilic cream, non-ionic...	275260	2
Bombastus	Hydrophilic cream, non-ionic...	275259	2
Bombastus	Hydrophilic cream, non-ionic...	271973	1
Bombastus	Hydrophilic cream, non-ionic...	278694	2
Caelo	Hydrophilic cream, non-ionic...	278694	1
Bombastus	Hydrophilic cream, non-ionic...	282904	1
Bombastus	Hydrophilic cream, non-ionic...	282903	1
Caelo	Hydrophilic cream, non-ionic...		1
Caelo	Hydrophilic cream, non-ionic...	4812I-02543	1
Caelo	Hydrophilic cream, non-ionic...	5112I-02543	1
Caelo	Hydrophilic cream, non-ionic...	CHB13263501	1
Caelo	Hydrophilic cream, non-ionic...	11273302	1
Noweda	Hydrophilic cream, non-ionic...	11357301	1
Caelo	Hydrophilic cream, non-ionic...	11357501	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Hydrophilic cream, non-ionic...	13138001	1

- 58 069 spectra from 332 *Apo-Ident* customers from a total of 19 968 batches from a further 328 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 cream, non-ionic DAB* 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 cream, non-ionic DAB* 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	310	0	34 034
Type B	0	814	146	62 634
Type C	0	282	90	58 069

The substance/substance group *Hydrophilic cream, non-ionic DAB* 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 % (> 99.9689 %)	100.0000 % (> 98.0645 %)
Type B	100.0000 % (> 99.9710 %)	84.7917 % (> 84.4792 %)
Type C	100.0000 % (> 99.5963 %)	75.8065 % (> 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.

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
31001	31748	8.85	18.03
31227	31748	7.05	17.98
31451	31451	0.00	15.90

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31748	31748	0.00	13.20
31749	31748	4.26	15.63
32088	32088	0.00	14.43
32105	31748	5.30	15.20
32726	31748	9.46	18.87

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Hydrophilic ointments
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30631-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydrophilic ointments; Anionic hydrophilic cream DAB; Anionic hydrophilic cream SR (NRF p.27); Anionic hydrophilic cream with propylene glycol; Anionic hydrophilic cream without preservatives; Base cream, hydrophobic DAC; Cremor anionicus hydrophilicus SR; Cremor basalis hydrophobicus; Cremor nonionicus hydrophilicus SR; Hydrophilic cream, non-ionic SR (NRF p.26); Hydrophilic cream, non-ionic without preservatives SR; Skin care ointment W/L SR; Skin care ointment W/L SR (without preservatives); Transdermal basic cream; Unguentum basale hydrophobicum; Unguentum emulsificans aquosum cum propylenglycolum; Unguentum emulsificans aquosum DAB; Unguentum emulsificans aquosum N sine conservante SR; Unguentum emulsificans aquosum N SR (NRF S. 26); Unguentum emulsificans aquosum sine conservante; Unguentum emulsificans aquosum SR (NRF S. 27); Wolff® basic half-fat cream

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 ointments*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Dr. Wolff	Wolff [®] basic hal...	230200	30631	50	20120210
Caelo	Base cream, hydr...	12151602	30758	40	20120612
Bombastus	Hydrophilic crea...	00273130	30769	40	1405255
Dr. Wolff	Wolff [®] basic hal...	236420	30837	40	1410330
Caelo	Anionic hydrophi...	12221002	30880	50	20120911
apomix	Anionic hydrophi...	25A210812	30895	60	20120821
Caelo	Base cream, hydr...	12308102	30931	40	20121031
Caelo	Base cream, hydr...	13085601	31002	40	20130404
Fagron	Transdermal basi...	12H17-T02-000281	31008	40	1406052
apomix	Skin care ointme...	01B110113	31039	40	1403321
apomix	Skin care ointme...	88B111212	31040	40	20121211
Fagron	Transdermal basi...	12H17-T02-000281	31042	40	20130110
Bombastus	Anionic hydrophi...	280574	31054	40	1405103
Dr. Wolff	Wolff [®] basic hal...	331551	31086	40	20130221
apomix	Hydrophilic crea...	21B141013	31188	40	1405386
Caelo	Anionic hydrophi...	13343401	31231	40	1403496
Caelo	Anionic hydrophi...	13244401	31241	30	20130726
Caelo	Anionic hydrophi...	14138901	31440	40	AR-15-FG-008131-01
Caelo	Anionic hydrophi...	14063303	31450	40	20140512
Caelo	Anionic hydrophi...	14030701	31470	40	20140204
Caelo	Hydrophilic crea...	14127002	31477	40	20140512
Caelo	Base cream, hydr...	14028101	31478	40	AR-15-FG-009038-01
Dr. Wolff	Wolff [®] basic hal...	432611	31487	40	20140410
apomix	Hydrophilic crea...	14B240614	31500	20	1411613
apomix	Skin care ointme...	10A050214	31503	40	1412041
apomix	Hydrophilic crea...	14B240614	31516	40	20140624
apomix	Anionic hydrophl...	11B020914	31537	40	1411614
apomix	Hydrophilic crea...	22B061114	31565	40	20141106
Bombastus	Hydrophilic crea...	288882	31568	40	20140722
Caelo	Hydrophilic crea...	14304902	31591	40	20141013
Fagron	Hydrophilic crea...	14E07-M04	31593	40	20140513
apomix	Hydrophilic crea...	01B120115	31599	40	20150114
apomix	Skin care ointme...	31B020714	31600	40	20140702
Pharmachem	Base cream, hydr...	150404	31644	40	20150306
apomix	Anionic hydrophl...	05B200415	31661	50	20150422
Caelo	Anionic hydrophi...	15048501	31741	40	9128
Caelo	Base cream, hydr...	15221202	31799	40	1605111
Caelo	Base cream, hydr...	154212	31906	40	20151211*
Caelo	Base cream, hydr...	154213	31907	40	20151211*
apomix	Hydrophilic crea...	25B081215	31962	40	20151209
Caelo	Hydrophilic crea...	153656	31996	40	20151211*
Caelo	Anionic hydrophi...	154004	32022	30	20151117*
Caelo	Anionic hydrophi...	153971	32039	40	20151113*
Caelo	Anionic hydrophi...	153573	32052	40	20151015*
Caelo	Anionic hydrophi...	153295	32123	40	20150924*
Caelo	Anionic hydrophi...	160673	32132	40	20160310*
Caelo	Anionic hydrophi...	160677	32142	40	20160310*
Pharmachem	Base cream, hydr...	160825	32303	40	20160517
Fagron	Transdermal basi...	15A28-T10-018922	32346	40	20150804
Caelo	Anionic hydrophi...	161525	32435	40	20160518*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

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

Type A All calibration spectra.

- 2010 spectra of 50 reference samples from the substance/substance group *Hydrophilic ointments*. These samples are listed above in the [calibration samples](#) section.
- 32334 spectra from a total of 750 batches from further 214 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 10693 spectra of 256 reference samples from the substance/substance group *Hydrophilic ointments*.

Supplier	Substance	Batch	Sample ID	Spectra
Bombastus	Base cream, hydrophobic DAC	234743	30219	40
zu erfassen	Anionic hydrophilic cream wit...	pending	30223	40
Bombastus	Hydrophilic cream, non-ionic...	258017	30233	40
Bombastus	Anionic hydrophilic cream DAB	263988	30333	40
Bombastus	Anionic hydrophilic cream SR...	262477	30337	40
apomix	Anionic hydrophilic cream SR...	24A080811	30349	20
apomix	Anionic hydrophilic cream wit...	15B111011	30350	30
apomix	Hydrophilic cream, non-ionic...	25A140911	30352	30
apomix	Hydrophilic cream, non-ionic...	27B111011	30353	30
apomix	Skin care ointment W/L SR	58B190711	30355	30
Leyh Pharma	Hydrophilic cream, non-ionic...	112311	30368	30
apomix	Hydrophilic cream, non-ionic...	1A030112	30392	40
Bombastus	Anionic hydrophilic cream DAB	266260	30402	40
Caelo	Anionic hydrophilic cream DAB	11225101	30404	40
Fagron	Hydrophilic cream, non-ionic...	34B191211	30440	40
Leyh Pharma	Hydrophilic cream, non-ionic...	120211	30441	40
apomix	Hydrophilic cream, non-ionic...	267186	30444	40
Caelo	Anionic hydrophilic cream DAB	11258201	30446	40
Caelo	Anionic hydrophilic cream DAB	11326601	30462	40
Caelo	Base cream, hydrophobic DAC	12025003	30467	60
Fagron	Hydrophilic cream, non-ionic...	9B190312	30483	40
Caelo	Anionic hydrophilic cream wi...	12117005	30572	40
Caelo	Anionic hydrophilic cream wi...	12117002	30577	80
Dr. Wolff	Wolff [®] basic half-fat cream	pending	30715	40
apomix	Skin care ointment W/L SR	10A050214	31503 [†]	20
apomix	Hydrophilic cream, non-ionic...	14B240614	31516 [†]	20
apomix	Anionic hydrophilic cream wit...	11B020914	31537 [†]	20
apomix	Hydrophilic cream, non-ionic...	22B061114	31565 [†]	20
Bombastus	Hydrophilic cream, non-ionic...	288882	31568 [†]	20
Caelo	Hydrophilic cream, non-ionic...	14304902	31591 [†]	20
Fagron	Hydrophilic cream, non-ionic...	14E07-M04	31593 [†]	20
apomix	Hydrophilic cream, non-ionic...	1B120115	31599 [†]	20
apomix	Skin care ointment W/L SR (w...	31B020714	31600 [†]	20
Pharmachem	Base cream, hydrophobic DAC	150404	31644 [†]	20

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Supplier	Substance	Batch	Sample ID	Spectra
apomix	Anionic hydrophilic cream wit...	5B200415	31661 [†]	20
Caelo	Anionic hydrophilic cream wi...	15048501	31741 [†]	20
Caelo	Base cream, hydrophobic DAC	15221202	31799 [†]	20
Caelo	Base cream, hydrophobic DAC	154212	31906 [†]	20
Caelo	Base cream, hydrophobic DAC	154213	31907 [†]	20
Caelo	Base cream, hydrophobic DAC	154214	31908	60
apomix	Hydrophilic cream, non-ionic...	25B081215	31962 [†]	20
Caelo	Hydrophilic cream, non-ionic...	160175	31994	60
Caelo	Hydrophilic cream, non-ionic...	153258	31995	60
Caelo	Anionic hydrophilic cream DAB	154004	32022 [†]	15
Caelo	Anionic hydrophilic cream DAB	154005	32023	60
Caelo	Anionic hydrophilic cream DAB	154007	32024	60
Caelo	Anionic hydrophilic cream DAB	154009	32025	60
Caelo	Anionic hydrophilic cream DAB	154012	32026	60
Caelo	Anionic hydrophilic cream DAB	154012	32027	60
Caelo	Anionic hydrophilic cream DAB	154013	32028	60
Caelo	Anionic hydrophilic cream DAB	154014	32029	60
Caelo	Anionic hydrophilic cream DAB	154015	32030	60
Caelo	Anionic hydrophilic cream DAB	154317	32031	60
Caelo	Anionic hydrophilic cream DAB	154317	32032	60
Caelo	Anionic hydrophilic cream DAB	154321	32033	60
Caelo	Anionic hydrophilic cream DAB	154321	32034	60
Caelo	Anionic hydrophilic cream DAB	153529	32035	60
Caelo	Anionic hydrophilic cream DAB	153530	32036	60
Caelo	Anionic hydrophilic cream DAB	153970	32037	60
Caelo	Anionic hydrophilic cream DAB	153971	32038	60
Caelo	Anionic hydrophilic cream DAB	153971	32039 [†]	20
Caelo	Anionic hydrophilic cream DAB	153972	32040	60
Caelo	Anionic hydrophilic cream DAB	153973	32041	60
Caelo	Anionic hydrophilic cream DAB	153575	32042	60
Caelo	Anionic hydrophilic cream DAB	153969	32043	60
Caelo	Anionic hydrophilic cream DAB	153969	32044	60
Caelo	Anionic hydrophilic cream DAB	154281	32045	60
Caelo	Anionic hydrophilic cream DAB	154282	32046	60
Caelo	Anionic hydrophilic cream DAB	154282	32047	60
Caelo	Anionic hydrophilic cream DAB	153531	32048	60
Caelo	Anionic hydrophilic cream DAB	153571	32049	60
Caelo	Anionic hydrophilic cream DAB	153572	32050	60
Caelo	Anionic hydrophilic cream DAB	153574	32051	60
Caelo	Anionic hydrophilic cream DAB	153573	32052 [†]	20
Caelo	Anionic hydrophilic cream DAB	153573	32053	60
Caelo	Anionic hydrophilic cream DAB	153575	32054	60
Caelo	Anionic hydrophilic cream DAB	154284	32055	60
Caelo	Anionic hydrophilic cream DAB	154284	32056	60
Caelo	Anionic hydrophilic cream DAB	153194	32057	60
Caelo	Anionic hydrophilic cream DAB	154281	32058	60
Caelo	Anionic hydrophilic cream DAB	154285	32059	60
Caelo	Anionic hydrophilic cream DAB	154285	32060	60
Caelo	Anionic hydrophilic cream DAB	154283	32061	60
Caelo	Anionic hydrophilic cream DAB	154283	32062	60
Caelo	Anionic hydrophilic cream DAB	153968	32063	60
Caelo	Anionic hydrophilic cream SR...	161075	32115	40
Caelo	Anionic hydrophilic cream SR...	161075	32116	40
Caelo	Hydrophilic cream, non-ionic...	161141	32119	40
Caelo	Hydrophilic cream, non-ionic...	161141	32120	40
Caelo	Hydrophilic cream, non-ionic...	161142	32121	40
Caelo	Hydrophilic cream, non-ionic...	161142	32122	40
Caelo	Anionic hydrophilic cream SR...	153296	32124	40
Caelo	Anionic hydrophilic cream SR...	153865	32125	40

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Anionic hydrophilic cream SR...	153866	32126	40
Caelo	Anionic hydrophilic cream SR...	160196	32127	40
Caelo	Anionic hydrophilic cream SR...	160198	32128	40
Caelo	Anionic hydrophilic cream wi...	160673	32129	40
Caelo	Anionic hydrophilic cream wi...	160673	32130	40
Caelo	Anionic hydrophilic cream wi...	160673	32131	40
Caelo	Anionic hydrophilic cream wi...	160674	32133	40
Caelo	Anionic hydrophilic cream wi...	160674	32134	40
Caelo	Anionic hydrophilic cream wi...	160674	32135	40
Caelo	Anionic hydrophilic cream wi...	160674	32136	40
Caelo	Anionic hydrophilic cream wi...	160675	32137	40
Caelo	Anionic hydrophilic cream wi...	160675	32138	40
Caelo	Anionic hydrophilic cream wi...	160676	32139	40
Caelo	Anionic hydrophilic cream wi...	160676	32140	40
Caelo	Anionic hydrophilic cream wi...	160677	32141	40
Caelo	Anionic hydrophilic cream wi...	160678	32143	40
Caelo	Anionic hydrophilic cream wi...	160679	32144	40
Caelo	Anionic hydrophilic cream DAB	160578	32145	40
Caelo	Anionic hydrophilic cream DAB	161031	32146	40
Caelo	Anionic hydrophilic cream DAB	161031	32147	40
Caelo	Anionic hydrophilic cream DAB	161033	32148	40
Caelo	Base cream, hydrophobic DAC	160748	32149	40
Caelo	Base cream, hydrophobic DAC	160748	32150	40
Caelo	Base cream, hydrophobic DAC	160749	32151	40
Caelo	Base cream, hydrophobic DAC	160749	32152	40
Caelo	Base cream, hydrophobic DAC	160751	32153	40
Caelo	Base cream, hydrophobic DAC	160751	32154	40
Caelo	Base cream, hydrophobic DAC	160750	32155	40
Caelo	Base cream, hydrophobic DAC	160752	32156	40
Caelo	Anionic hydrophilic cream DAB	161510	32218	40
Caelo	Anionic hydrophilic cream DAB	161510	32219	40
Caelo	Anionic hydrophilic cream DAB	161507	32220	40
Caelo	Anionic hydrophilic cream DAB	161507	32221	40
Caelo	Anionic hydrophilic cream DAB	161508	32222	40
Caelo	Anionic hydrophilic cream SR...	161267	32225	40
Caelo	Base cream, hydrophobic DAC	160750	32226	40
Caelo	Base cream, hydrophobic DAC	161654	32370	41
Caelo	Base cream, hydrophobic DAC	161654	32371	41
Caelo	Base cream, hydrophobic DAC	161655	32372	41
Caelo	Base cream, hydrophobic DAC	161655	32373	41
Caelo	Base cream, hydrophobic DAC	161656	32374	41
Caelo	Base cream, hydrophobic DAC	161656	32375	40
Caelo	Base cream, hydrophobic DAC	161657	32376	41
Caelo	Base cream, hydrophobic DAC	161657	32377	41
Caelo	Base cream, hydrophobic DAC	161742	32378	41
Caelo	Hydrophilic cream, non-ionic...	161694	32382	40
Caelo	Hydrophilic cream, non-ionic...	161694	32383	40
Caelo	Hydrophilic cream, non-ionic...	161695	32384	40
Caelo	Hydrophilic cream, non-ionic...	161695	32385	40
Caelo	Anionic hydrophilic cream SR...	162155	32386	40
Caelo	Anionic hydrophilic cream SR...	162156	32387	40
Caelo	Anionic hydrophilic cream SR...	162157	32388	40
Caelo	Anionic hydrophilic cream wi...	161918	32422	40
Caelo	Anionic hydrophilic cream wi...	161918	32423	40
Caelo	Anionic hydrophilic cream wi...	161919	32424	40
Caelo	Anionic hydrophilic cream wi...	161919	32425	40
Caelo	Anionic hydrophilic cream DAB	161506	32426	40
Caelo	Anionic hydrophilic cream DAB	161506	32427	40
Caelo	Anionic hydrophilic cream DAB	161506	32428	40
Caelo	Anionic hydrophilic cream DAB	161510	32429	40

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Anionic hydrophilic cream DAB	161510	32430	40
Caelo	Anionic hydrophilic cream DAB	161798	32431	40
Caelo	Anionic hydrophilic cream DAB	161798	32432	40
Caelo	Anionic hydrophilic cream DAB	161798	32433	40
Caelo	Anionic hydrophilic cream DAB	161798	32434	40
Caelo	Anionic hydrophilic cream DAB	161525	32436	40
Caelo	Anionic hydrophilic cream DAB	161529	32437	40
Caelo	Anionic hydrophilic cream DAB	161529	32438	40
Caelo	Anionic hydrophilic cream DAB	161529	32439	40
Caelo	Anionic hydrophilic cream DAB	161526	32440	40
Caelo	Anionic hydrophilic cream DAB	161526	32441	40
Caelo	Anionic hydrophilic cream DAB	161526	32442	40
Caelo	Anionic hydrophilic cream DAB	161526	32443	40
Caelo	Anionic hydrophilic cream DAB	161527	32444	40
Caelo	Anionic hydrophilic cream DAB	161527	32445	40
Caelo	Anionic hydrophilic cream DAB	161527	32446	40
Caelo	Anionic hydrophilic cream DAB	161528	32447	40
Caelo	Anionic hydrophilic cream DAB	161528	32448	40
Caelo	Anionic hydrophilic cream DAB	161528	32449	40
Caelo	Anionic hydrophilic cream DAB	161560	32450	40
Caelo	Anionic hydrophilic cream DAB	161561	32451	40
Caelo	Anionic hydrophilic cream DAB	161563	32452	40
Caelo	Anionic hydrophilic cream DAB	161564	32453	40
Caelo	Base cream, hydrophobic DAC	161654	32491	40
Caelo	Base cream, hydrophobic DAC	161655	32492	40
Caelo	Base cream, hydrophobic DAC	161742	32508	40
Caelo	Base cream, hydrophobic DAC	161656	32509	40
Caelo	Base cream, hydrophobic DAC	161657	32510	40
Caelo	Anionic hydrophilic cream SR...	162586	32550	40
Caelo	Anionic hydrophilic cream SR...	162587	32551	40
Caelo	Anionic hydrophilic cream SR...	162587	32552	40
Caelo	Anionic hydrophilic cream SR...	162587	32553	40
Caelo	Hydrophilic cream, non-ionic...	161694	32582	40
Caelo	Hydrophilic cream, non-ionic...	161695	32583	40
Caelo	Hydrophilic cream, non-ionic...	162220	32584	40
Caelo	Hydrophilic cream, non-ionic...	162220	32585	40
Caelo	Hydrophilic cream, non-ionic...	162220	32594	40
Caelo	Hydrophilic cream, non-ionic...	162220	32595	40
Caelo	Hydrophilic cream, non-ionic...	162221	32596	40
Caelo	Hydrophilic cream, non-ionic...	162221	32597	40
Caelo	Hydrophilic cream, non-ionic...	162221	32598	40
Caelo	Hydrophilic cream, non-ionic...	162221	32599	40
Caelo	Hydrophilic cream, non-ionic...	162221	32600	40
Caelo	Hydrophilic cream, non-ionic...	162221	32601	40
Caelo	Hydrophilic cream, non-ionic...	162579	32602	40
Caelo	Hydrophilic cream, non-ionic...	162579	32603	40
Caelo	Anionic hydrophilic cream wi...	161915	32619	40
Caelo	Anionic hydrophilic cream wi...	161916	32620	40
Caelo	Anionic hydrophilic cream wi...	161917	32621	40
Caelo	Anionic hydrophilic cream wi...	161918	32622	40
Caelo	Anionic hydrophilic cream wi...	161919	32623	40
Caelo	Anionic hydrophilic cream DAB	161561	32642	40
Caelo	Anionic hydrophilic cream DAB	161563	32643	40
Caelo	Anionic hydrophilic cream DAB	161589	32644	40
Caelo	Anionic hydrophilic cream DAB	161796	32645	40
Caelo	Anionic hydrophilic cream DAB	161796	32646	40
Caelo	Anionic hydrophilic cream DAB	161797	32647	40
Caelo	Anionic hydrophilic cream DAB	161800	32648	40
Caelo	Anionic hydrophilic cream DAB	162500	32649	40
Caelo	Anionic hydrophilic cream DAB	162500	32650	40

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Anionic hydrophilic cream DAB	162501	32651	40
Caelo	Anionic hydrophilic cream DAB	162501	32652	40
Caelo	Anionic hydrophilic cream DAB	162502	32653	40
Caelo	Anionic hydrophilic cream DAB	162589	32654	40
Caelo	Anionic hydrophilic cream DAB	162589	32655	40
Caelo	Anionic hydrophilic cream DAB	162590	32656	40
Caelo	Anionic hydrophilic cream DAB	162590	32657	40
Caelo	Anionic hydrophilic cream DAB	162591	32658	40
Caelo	Anionic hydrophilic cream DAB	162591	32659	40
Caelo	Anionic hydrophilic cream DAB	162591	32660	40
Caelo	Anionic hydrophilic cream DAB	162592	32661	40
Caelo	Anionic hydrophilic cream DAB	162592	32662	40
Caelo	Anionic hydrophilic cream DAB	162593	32663	40
Caelo	Anionic hydrophilic cream DAB	162593	32664	40
Caelo	Anionic hydrophilic cream DAB	162593	32665	40
Caelo	Anionic hydrophilic cream DAB	162593	32666	40
Caelo	Anionic hydrophilic cream DAB	162594	32667	40
Caelo	Anionic hydrophilic cream DAB	162594	32668	40
Caelo	Anionic hydrophilic cream DAB	162596	32669	40
Caelo	Anionic hydrophilic cream DAB	162596	32670	40
Caelo	Anionic hydrophilic cream DAB	162596	32671	40
Caelo	Anionic hydrophilic cream DAB	162597	32672	40
Caelo	Anionic hydrophilic cream DAB	162597	32673	40
Caelo	Anionic hydrophilic cream DAB	162599	32674	40
Caelo	Anionic hydrophilic cream DAB	162599	32675	40
Caelo	Anionic hydrophilic cream DAB	162600	32676	40
Caelo	Anionic hydrophilic cream DAB	162600	32677	40
Caelo	Anionic hydrophilic cream DAB	162645	32678	40
Caelo	Base cream, hydrophobic DAC	162937	32855	40
Caelo	Base cream, hydrophobic DAC	162938	32856	40
Caelo	Base cream, hydrophobic DAC	162939	32857	40
Caelo	Anionic hydrophilic cream DAB	162643	32875	40
Caelo	Anionic hydrophilic cream DAB	162644	32876	40
Caelo	Anionic hydrophilic cream DAB	162646	32877	40
Caelo	Anionic hydrophilic cream DAB	162647	32878	40
Caelo	Anionic hydrophilic cream DAB	162598	32879	40
Caelo	Anionic hydrophilic cream DAB	163172	32880	40
Caelo	Anionic hydrophilic cream DAB	163226	32881	40
Caelo	Anionic hydrophilic cream wi...	162901	32882	40
Caelo	Anionic hydrophilic cream wi...	162902	32883	40
Caelo	Anionic hydrophilic cream wi...	162903	32884	40
Caelo	Anionic hydrophilic cream wi...	162904	32885	40
Caelo	Anionic hydrophilic cream wi...	162905	32886	40

- 52901 spectra from a total of 1315 batches from further 430 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.

[†]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*.

- 5986 spectra from 296 *Apo-Ident* customers from 2124 batches from the substance/substance group *Hydrophilic ointments*.

Supplier	Substance	Batch	Spectra
AMH Niemann/G	Anionic hydrophlic cream wit...	1B070114	1
Caelo	Anionic hydrophilic cream SR...	2091403	1
AMH Niemann / Noweda	Anionic hydrophlic cream wit...	1B070114	1
Bombastus	Anionic hydrophilic cream SR...	292980	2
AMH Niemann / G	Anionic hydrophilic cream SR...	2A130114	1
AMH Niemann / G	Anionic hydrophilic cream SR...	3A200115	1
Caelo	Anionic hydrophilic cream SR...	4061406	1
Gehe/Apomix	Anionic hydrophilic cream SR...	4A030214	2
apomix/Noweda	Anionic hydrophlic cream wit...	2B250116	1
AMH Niemann / G	Anionic hydrophlic cream wit...	4B100314	1
APOMIX/Noweda	Anionic hydrophlic cream wit...	4B210316	1
AMH Niemann GmbH&Co.KG	Anionic hydrophlic cream wit...	3B020315	1
AMH Niemann / E	Anionic hydrophilic cream SR...	4A030214	1
Apomix/Noweda	Anionic hydrophilic cream SR...	4A270115	1
Gehe	Anionic hydrophlic cream wit...	2B100214	1
Apomix/Noweda	Anionic hydrophlic cream wit...	3B240214	1
apomix/Phönix	Anionic hydrophlic cream wit...	4B250315	1
Apomix/Noweda	Anionic hydrophlic cream wit...	5B070414	1
Caelo	Anionic hydrophilic cream SR...	6061502	1
Apomix	Anionic hydrophlic cream wit...	6B040515	1
Apomix/Noweda	Anionic hydrophlic cream wit...	6B040515	1
Apomix	Anionic hydrophlic cream wit...	6B04515	1
apomix/Noweda	Anionic hydrophlic cream wit...	6B060514	1
PKH Halle / Phoenix	Anionic hydrophilic cream SR...	5A170214	1
AMH Niemann / G	Anionic hydrophlic cream wit...	6B060514	1
APOMIX/Noweda	Anionic hydrophilic cream SR...	7a090216	1
AMH Niemann / G	Anionic hydrophlic cream wit...	7B080615	1
Apomix/Noweda	Anionic hydrophlic cream wit...	9B130715	1
AMH Niemann / G	Anionic hydrophlic cream wit...	10B060814	1
AMH Niemann / G	Anionic hydrophilic cream SR...	10A050315	1
apomix/GEHE/28.05.14	Anionic hydrophilic cream SR...	11A010414	1
Pharmachem/Phönix	Anionic hydrophilic cream SR...	110913	1
apomix/Phönix	Anionic hydrophilic cream SR...	11A010316	1
Apomix/Noweda	Anionic hydrophilic cream SR...	8A260314	1
Caelo	Anionic hydrophilic cream DAB	12345	1
Apomix/Noweda	Anionic hydrophlic cream wit...	9B220714	1
Caelo	Anionic hydrophilic cream DAB	123test	1
Raben-Apotheke Mildenau	Anionic hydrophilic cream SR...	11A010414	1
apomix/Phönix	Anionic hydrophilic cream SR...	12A3103215	1
Caelo	Anionic hydrophilic cream SR...	11A010414	1
AMH Niemann / G	Anionic hydrophilic cream SR...	11A010414	1
Apomix/Noweda	Anionic hydrophilic cream SR...	12A310315	1
apomix/Phönix	Anionic hydrophilic cream SR...	12A310315	1
Apomix/Noweda	Anionic hydrophlic cream wit...	12B212015	1
Apomix/Noweda	Anionic hydrophlic cream wit...	12B220914	1
Apomix	Anionic hydrophlic cream wit...	12B220914	2
AMH Niemann / G	Anionic hydrophilic cream SR...	12A310315	1
Pharmachem/Phönix	Anionic hydrophilic cream SR...	130814	1
PKH Halle	Anionic hydrophilic cream SR...	13A010415	1
apomix/Phönix	Anionic hydrophlic cream wit...	13B161115	1
Apomix/Noweda	Anionic hydrophilic cream SR...	13A080414	1
Caelo	Anionic hydrophilic cream SR...	14063303	2
Caelo	Anionic hydrophilic cream SR...	14041403	1
Caelo	Anionic hydrophilic cream SR...	14186501	2
Caelo	Anionic hydrophilic cream SR...	14182101	1
Caelo	Anionic hydrophilic cream SR...	14244701	3

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Supplier	Substance	Batch	Spectra
Caelo	Anionic hydrophilic cream SR...	14301501	6
Caelo	Anionic hydrophilic cream SR...	14336203	2
Caelo	Anionic hydrophilic cream SR...	15014801	2
Gehe	Anionic hydrophilic cream SR...	15014804	1
Caelo	Anionic hydrophilic cream SR...	15014804	1
Caelo	Anionic hydrophilic cream SR...	15069501	2
Caelo	Anionic hydrophilic cream SR...	15172901	4
Caelo	Anionic hydrophilic cream SR...	15134602	2
Caelo	Anionic hydrophilic cream SR...	15069403	1
Caelo	Anionic hydrophilic cream SR...	15268001	1
Caelo	Anionic hydrophilic cream SR...	15329501	5
Caelo	Anionic hydrophilic cream SR...	15205501	2
Caelo	Anionic hydrophilic cream wi...	15272902	3
Caelo	Anionic hydrophilic cream SR...	15268002	1
Caelo	Anionic hydrophilic cream SR...	15329601	6
Noweda	Anionic hydrophilic cream SR...	15329601	1
Caelo	Anionic hydrophilic cream wi...	15405302	2
Noweda	Anionic hydrophilic cream SR...	15386502	1
Caelo	Anionic hydrophilic cream SR...	15386602	1
Caelo	Anionic hydrophilic cream SR...	15386502	1
Caesar&Loretz GmbH	Anionic hydrophilic cream SR...	15386602	1
Caelo	Anionic hydrophilic cream DAB	15428501	3
Caesar & Loretz GmbH Hi...	Anionic hydrophilic cream DAB	15432001	2
Apomix/Noweda	Anionic hydrophlic cream wit...	15B291214	1
PKH / Phoenix	Anionic hydrophilic cream SR...	15A210415	1
Caelo	Anionic hydrophilic cream SR...	160107502	1
Caesar&Loretz GmbH	Anionic hydrophilic cream SR...	16019601	1
Caelo	Anionic hydrophilic cream SR...	16019801	3
Caelo	Anionic hydrophilic cream DAB	16046201	5
Caelo	Anionic hydrophilic cream DAB	16046901	5
Caelo	Anionic hydrophlic cream wit...	16047001	1
Caelo	Anionic hydrophilic cream DAB	160470001	1
Caelo	Anionic hydrophilic cream DAB	16047001	4
Caelo	Anionic hydrophilic cream DAB	16057701	3
Caelo	Anionic hydrophilic cream DAB	16057601	2
Caelo	Anionic hydrophilic cream DAB	16057501	3
Caelo	Anionic hydrophilic cream DAB	16057901	2
Caelo	Anionic hydrophilic cream DAB	16058001	2
Gehe	Anionic hydrophilic cream wi...	16067401	1
Caelo	Anionic hydrophilic cream wi...	16067501	4
Caelo	Anionic hydrophilic cream wi...	16067601	13
Bombastus	Anionic hydrophilic cream wi...	16067701	2
Caelo	Anionic hydrophilic cream wi...	16067801	3
Caelo	Anionic hydrophilic cream DAB	16103301	6
Martinus-Apotheke	Anionic hydrophilic cream wi...	16067801	1
Caelo	Anionic hydrophilic cream DAB	16103401	3
Caelo	Anionic hydrophilic cream wi...	16067901	2
Caelo	Anionic hydrophilic cream DAB	16103501	3
Fagron	Anionic hydrophilic cream DAB	16103501	1
Caelo	Anionic hydrophilic cream DAB	16103101	1
Cealo/AHD	Anionic hydrophilic cream SR...	16107501	1
Caelo	Anionic hydrophilic cream SR...	16107501	6
Caelo	Anionic hydrophilic cream SR...	16107502	1
Caesar&Loretz GmbH	Anionic hydrophilic cream SR...	16107502	1
Caelo	Anionic hydrophilic cream DAB	16150702	1
Euro OTC	Anionic hydrophilic cream DAB	16150801	1
Caelo	Anionic hydrophilic cream DAB	16150801	4
Caelo	Anionic hydrophilic cream DAB	16150703	1
Caelo	Anionic hydrophilic cream SR...	16150901	3
Caelo	Anionic hydrophilic cream DAB	16152501	1

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Supplier	Substance	Batch	Spectra
Caelo	Anionic hydrophilic cream DAB	16152701	6
Caelo	Anionic hydrophilic cream DAB	16152801	4
Caelo	Anionic hydrophilic cream DAB	16152901	1
Caelo	Anionic hydrophilic cream DAB	16156001	3
Caelo	Anionic hydrophilic cream DAB	16156101	6
Noweda	Anionic hydrophilic cream DAB	16156401	2
Caelo	Anionic hydrophilic cream DAB	16158701	5
Caelo	Anionic hydrophilic cream DAB	16158901	6
Caelo	Anionic hydrophilic cream DAB	16156401	4
Caesar & Loretz/Noweda	Anionic hydrophilic cream DAB	16158901	1
Caelo	Anionic hydrophilic cream DAB	16158803	1
Gehe	Anionic hydrophilic cream DAB	16179601	1
Caelo	Anionic hydrophilic cream DAB	16179702	2
Caelo	Anionic hydrophilic cream DAB	16179801	4
Phoenix	Anionic hydrophilic cream SR...	16188903	1
Caelo	Anionic hydrophilic cream DAB	16180001	4
Gehe	Anionic hydrophilic cream wi...	16191501	1
Caelo	Anionic hydrophilic cream wi...	16191601	5
Caelo	Anionic hydrophilic cream wi...	16191701	2
Caelo	Anionic hydrophilic cream wi...	16191901	1
Caelo	Anionic hydrophilic cream wi...	16191801	1
Caelo	Anionic hydrophilic cream SR...	162115501	1
Caelo	Anionic hydrophilic cream DAB	16249902	1
Caelo	Anionic hydrophilic cream DAB	16220201	1
Calo/Sanacorp	Anionic hydrophilic cream DAB	16259302	1
Caelo	Anionic hydrophilic cream DAB	16259901	2
Caelo	Anionic hydrophilic cream DAB	16250201	5
Caelo	Anionic hydrophilic cream DAB	16264301	3
AMH Niemann / E	Anionic hydrophilic cream SR...	16A050515	1
Apomix	Anionic hydrophilic cream SR...	18A040516	1
PKH/Gehe	Anionic hydrophilic cream SR...	16A060416	1
Apomix/Noweda	Anionic hydrophilic cream SR...	18A260514	1
apomix/Gehe	Anionic hydrophilic cream SR...	18A260514	2
PKH Halle / Phoenix	Anionic hydrophilic cream SR...	17A200514	1
Apomix/Sanacorp	Anionic hydrophilic cream SR...	17A030516	1
All..Healthc./Apomix	Anionic hydrophilic cream SR...	18A260514	1
Gehe/Apomix	Anionic hydrophilic cream SR...	16A130514	1
Raben-Apotheke Mildenau	Anionic hydrophilic cream SR...	19A030614	1
Apomix/Gehe	Anionic hydrophilic cream SR...	19A260515	2
apomix/Gehe	Anionic hydrophilic cream SR...	19A030614	1
Gehe/apomix/23.09.14	Anionic hydrophilic cream SR...	19A030614	1
Apomix/Noweda	Anionic hydrophilic cream SR...	20A020615	2
AMH Niemann / E	Anionic hydrophilic cream SR...	20A020615	1
Noweda/apomix	Anionic hydrophilic cream SR...	21A090615	1
Apomix/Phönix	Anionic hydrophilic cream SR...	21A180614	1
Bombastus	Anionic hydrophilic cream SR...	2215M-03327	1
Caelo	Anionic hydrophilic cream SR...	22A160615	2
Caelo	Anionic hydrophilic cream SR...	23121411	1
Neidhardt	Anionic hydrophilic cream SR...	25A140714	1
Gehe/02.09.14/apomix	Anionic hydrophilic cream SR...	23A240614	1
Euro OTC	Anionic hydrophilic cream DAB	260416v2	1
apomix/AHD	Anionic hydrophilic cream SR...	24A280616	1
Pharmachem/Phoenix	Anionic hydrophilic cream SR...	260712	3
Gehe/apomix/17.12.2014	Anionic hydrophilic cream SR...	26A060814	1
apomix/Phönix	Anionic hydrophilic cream SR...	25A290616	1
Bombastus	Anionic hydrophilic cream SR...	280568	2
Bombastus	Anionic hydrophilic cream SR...	281738	8
apomix/Holdermann	Anionic hydrophilic cream SR...	26A130716	1
Bombastus	Anionic hydrophilic cream SR...	281767	6
Bombastus	Anionic hydrophilic cream SR...	283283	3

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Supplier	Substance	Batch	Spectra
Bombastus	Anionic hydrophilic cream SR...	281866	6
Bombastu-Werke AG/Gehe	Anionic hydrophilic cream SR...	281866	2
Bombastus	Anionic hydrophilic cream SR...	283279	2
Bombastus	Anionic hydrophilic cream SR...	283286	2
Bombastus	Anionic hydrophilic cream SR...	283285	4
Bombastus	Anionic hydrophilic cream SR...	284080	3
Bombastu-Werke AG/Gehe	Anionic hydrophilic cream SR...	283286	1
Bombastus	Anionic hydrophilic cream SR...	284082	3
Bombastus	Anionic hydrophilic cream SR...	284081	5
Bombastus	Anionic hydrophilic cream SR...	284083	4
Phönix	Anionic hydrophilic cream SR...	284083	1
Bombastus	Anionic hydrophilic cream SR...	285894	2
Bombastus	Anionic hydrophilic cream SR...	285893	2
Bombastus	Anionic hydrophilic cream SR...	285895	3
Bombastus	Anionic hydrophilic cream SR...	285892	1
Bombastus	Anionic hydrophilic cream wit...	285829	1
Bombastus	Anionic hydrophilic cream SR...	285890	2
Bombastus	Anionic hydrophilic cream SR...	285896	2
Bombastus	Anionic hydrophilic cream SR...	285897	2
Bombastus	Anionic hydrophilic cream SR...	285898	7
Bombastus	Anionic hydrophilic cream SR...	285899	4
Cealo	Anionic hydrophilic cream SR...	285899	1
Euro OTC	Anionic hydrophilic cream SR...	286838	2
Bombastus	Anionic hydrophilic cream SR...	286973	1
Gehe	Anionic hydrophilic cream SR...	286974	1
Euro OTC	Anionic hydrophilic cream SR...	286975	1
Bombastus	Anionic hydrophilic cream SR...	286975	3
Caelo	Anionic hydrophilic cream SR...	286976	2
Bombastus	Anionic hydrophilic cream SR...	286979	10
Bombastu-Werke AG/Gehe	Anionic hydrophilic cream SR...	286979	1
Caelo	Anionic hydrophilic cream SR...	286979	1
Bombastus	Anionic hydrophilic cream SR...	286980	8
Bombastus	Anionic hydrophilic cream SR...	288230	2
Bombastus	Anionic hydrophilic cream SR...	288234	2
Caelo	Anionic hydrophilic cream SR...	288235	1
Bombastus	Anionic hydrophilic cream SR...	288227	1
Bombastus	Anionic hydrophilic cream SR...	287717	1
Bombastus	Anionic hydrophilic cream SR...	288235	2
Caelo	Anionic hydrophilic cream SR...	288307	2
Bombastus	Anionic hydrophilic cream SR...	288233	1
Bombastus	Anionic hydrophilic cream SR...	288307	6
Bombastus	Anionic hydrophilic cream SR...	288308	3
Caelo	Anionic hydrophilic cream SR...	288310	1
Bombastus	Anionic hydrophilic cream SR...	288308	1
Bombastus	Anionic hydrophilic cream SR...	288310	4
Bombastus	Anionic hydrophilic cream SR...	289322	1
Bombastus	Anionic hydrophilic cream SR...	289325	1
Bombastus	Anionic hydrophilic cream SR...	289326	1
Bombastus	Anionic hydrophilic cream SR...	288882	1
Bombastus	Anionic hydrophilic cream SR...	289327	4
Bombastus	Anionic hydrophilic cream SR...	289328	2
Caelo	Anionic hydrophilic cream SR...	289331	1
Bombastus	Anionic hydrophilic cream SR...	289330	2
Bombastus	Anionic hydrophilic cream SR...	289331	3
Caelo	Anionic hydrophilic cream SR...	289332	1
Bombastus	Anionic hydrophilic cream SR...	289332	2
apomix/Phönix	Anionic hydrophilic cream SR...	28A040815	2
Apomix	Anionic hydrophilic cream SR...	28A190814	1
Apomix/Gehe	Anionic hydrophilic cream SR...	28A040815	1
apomix	Anionic hydrophilic cream SR...	28A190814	1

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Supplier	Substance	Batch	Spectra
Bombastus	Anionic hydrophilic cream SR...	290522	1
Bombastus	Anionic hydrophilic cream SR...	290523	2
Bombastus	Anionic hydrophilic cream SR...	290524	1
Bombastus	Anionic hydrophilic cream SR...	290525	1
Bombastus	Anionic hydrophilic cream SR...	290528	1
Dr. Wolff	Anionic hydrophilic cream SR...	290528	1
Bombastus	Anionic hydrophilic cream SR...	290530	5
Sanacorp	Anionic hydrophilic cream SR...	290530	1
Bombastus	Anionic hydrophilic cream SR...	291526	2
Bombastus	Anionic hydrophilic cream SR...	291523	3
Bombastus	Anionic hydrophilic cream SR...	291528	7
Bombastus	Anionic hydrophilic cream SR...	291525	2
Fagron	Anionic hydrophilic cream SR...	291528	1
Bombastus	Anionic hydrophilic cream SR...	291529	3
Bombastus	Anionic hydrophilic cream SR...	292975	2
Bombastus	Anionic hydrophilic cream SR...	292976	4
Bombastus	Anionic hydrophilic cream SR...	292977	1
Bombastus	Anionic hydrophilic cream SR...	292978	3
Bombastus	Anionic hydrophilic cream SR...	292979	3
Bombastus	Anionic hydrophilic cream SR...	293102	2
Bombastus	Anionic hydrophilic cream SR...	293103	1
Caelo	Anionic hydrophilic cream SR...	293103	1
Bombastus	Anionic hydrophilic cream SR...	293104	2
Bombast/Phoenix	Anionic hydrophilic cream SR...	293104	1
Caelo	Anionic hydrophilic cream SR...	293104	2
Bombastus	Anionic hydrophilic cream SR...	293133	1
Bombastus	Anionic hydrophilic cream SR...	293135	7
Caelo	Anionic hydrophilic cream SR...	293135	1
Bombastus	Anionic hydrophilic cream SR...	295166	3
Fagron	Anionic hydrophilic cream SR...	295166	2
Bombastus	Anionic hydrophilic cream SR...	295167	5
Bombastus	Anionic hydrophilic cream SR...	295232	2
Bombastus	Anionic hydrophilic cream SR...	295171	1
Bombastus	Anionic hydrophilic cream SR...	295233	2
Bombastus	Anionic hydrophilic cream SR...	295169	3
Bombastus	Anionic hydrophilic cream SR...	295170	1
Bombastus	Anionic hydrophilic cream SR...	296406	1
Caelo	Anionic hydrophilic cream SR...	296408	1
Euro OTC	Anionic hydrophilic cream SR...	296410	2
Bombastus	Anionic hydrophilic cream SR...	296412	2
Bombastus	Anionic hydrophilic cream SR...	296411	2
Bombastus	Anionic hydrophilic cream SR...		1
Bombastus	Anionic hydrophilic cream SR...	296413	1
Bombastus	Anionic hydrophilic cream SR...	296414	7
Bombastus	Anionic hydrophilic cream SR...	296415	2
Bombastus	Anionic hydrophilic cream SR...	297820	1
Bombastus	Anionic hydrophilic cream SR...	297821	3
Bombastus	Anionic hydrophilic cream SR...	297817	1
Bombastus	Anionic hydrophilic cream SR...	297822	4
Bombastus	Anionic hydrophilic cream SR...	297823	3
Bombastus	Anionic hydrophilic cream SR...	297909	1
Bombastus	Anionic hydrophilic cream SR...	297911	2
Caelo	Anionic hydrophilic cream SR...	297912	3
Bombastus	Anionic hydrophilic cream SR...	297913	5
Anzag	Anionic hydrophilic cream SR...	297911	2
Bombastus	Anionic hydrophilic cream SR...	299253	3
Bombastus	Anionic hydrophilic cream DAB	299256	1
Apomix	Anionic hydrophilic cream SR...	29A020914	1
AMH Niemann / G	Anionic hydrophilic cream SR...	29A020914	1
Bombastus	Anionic hydrophilic cream DAB	300350	1

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Supplier	Substance	Batch	Spectra
Bombastus	Anionic hydrophilic cream SR...	2x297819	1
Caelo	Anionic hydrophilic cream SR...	30011503	1
Bombastus	Anionic hydrophilic cream DAB	300352	1
Bombastus	Anionic hydrophilic cream DAB	300363	1
Bombastus	Anionic hydrophilic cream DAB	300353	1
Bombastus	Anionic hydrophilic cream DAB	300361	1
Bombastus	Anionic hydrophilic cream SR...	300561	1
Bombastus	Anionic hydrophilic cream DAB	300358	2
Bombastus	Anionic hydrophilic cream DAB	300365	1
Bombastus	Anionic hydrophilic cream SR...	300562	1
Bombastus	Anionic hydrophilic cream SR...	300564	7
Euro OTC	Anionic hydrophilic cream SR...	300563	1
Bombastus	Anionic hydrophilic cream DAB	300357	1
Bombastus	Anionic hydrophilic cream SR...	300563	2
Bombastus	Anionic hydrophilic cream SR...	300560	1
Bombastus	Anionic hydrophilic cream SR...	300947	1
Bombastus	Anionic hydrophilic cream SR...	300953	3
Bombastus	Anionic hydrophilic cream SR...	300955	2
Bombastus	Anionic hydrophilic cream SR...	300957	5
Bombastus	Anionic hydrophilic cream SR...	300956	2
Caelo	Anionic hydrophilic cream SR...	300956	1
Bombastus	Anionic hydrophilic cream DAB	301267	2
Bombastus	Anionic hydrophilic cream DAB	301270	1
Bombastus	Anionic hydrophilic cream DAB	301350	1
Bombastus	Anionic hydrophilic cream SR...	301352	1
Bombastus	Anionic hydrophilic cream DAB	301357	2
Caelo	Anionic hydrophilic cream SR...	302196	2
Bombastus	Anionic hydrophilic cream DAB	301358	1
Bombastus	Anionic hydrophilic cream SR...	302190	1
Bombastus	Anionic hydrophilic cream SR...	302192	1
Bombastus	Anionic hydrophilic cream SR...	302194	2
Bombastus	Anionic hydrophilic cream SR...	302196	1
Bombastus	Anionic hydrophilic cream SR...	302195	2
Euro OTC	Anionic hydrophilic cream SR...	302199	1
Bombastus	Anionic hydrophilic cream SR...	302199	2
Caelo	Anionic hydrophilic cream SR...	302200	1
Bombastus	Anionic hydrophilic cream DAB	302456	1
Bombastus	Anionic hydrophilic cream SR...	302200	2
Fagron	Anionic hydrophilic cream SR...	302382	1
Bombastus	Anionic hydrophilic cream DAB	302461	1
Bombastus	Anionic hydrophilic cream DAB	302463	1
Bombastus	Anionic hydrophilic cream DAB	302467	1
Bombastus	Anionic hydrophilic cream SR...	303735	3
Bombastus	Anionic hydrophilic cream SR...	303736	1
Bombastus	Anionic hydrophilic cream DAB	304094	1
Bombastus	Anionic hydrophilic cream SR...	305067	1
Noweda/Apomix	Anionic hydrophilic cream SR...	31A14014	1
AMH Niemann / G	Anionic hydrophilic cream SR...	31A230914	1
apomix/Gehe	Anionic hydrophilic cream SR...	31A230914	2
Apomix/Noweda	Anionic hydrophilic cream SR...	33A141014	1
Caelo	Anionic hydrophilic cream SR...	31A230914	1
apomix/Phönix	Anionic hydrophilic cream SR...	37A171115	1
Anzag/apomix/07.01.15	Anionic hydrophilic cream SR...	35A031114	1
apomix/Phönix	Anionic hydrophilic cream SR...	34A130916	1
Apomix/Noweda	Anionic hydrophilic cream SR...	37A17115	1
Rabenapotheke	Anionic hydrophilic cream SR...	39A011214	1
PKH Apomix/Anzag	Anionic hydrophilic cream SR...	38A171115	1
Apomix	Anionic hydrophilic cream SR...	39A011214	2
apomix/Gehe	Anionic hydrophilic cream SR...	41A101214	1
PKH Halle / Phoenix	Anionic hydrophilic cream SR...	40A091214	1

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Supplier	Substance	Batch	Spectra
Apomix/Noweda	Anionic hydrophilic cream SR...	42A171214	1
Bombastus	Anionic hydrophilic cream SR...	98245	1
AMH Niemann/E	Anionic hydrophilic cream SR...	45A141113	1
Gehe/Apomix	Anionic hydrophilic cream SR...	48A031213	1
Gehe 10.03.15	Anionic hydrophilic cream SR...	42A171214	1
AMH Niemann / G	Anionic hydrophilic cream SR...	41A101214	1
Apomix	Anionic hydrophilic cream SR...	42A171214	2
Bombastus	Anionic hydrophilic cream SR...	244379	1
Bombastus	Anionic hydrophilic cream SR...	258517	1
Caelo	Anionic hydrophilic cream wit...		1
Caelo	Anionic hydrophilic cream wi...		1
Bombastus	Anionic hydrophilic cream SR...	229317	1
Bombastus	Anionic hydrophilic cream SR...	261013	2
Caelo	Anionic hydrophilic cream DAB	Mh090716Lo1	1
Gehe	Anionic hydrophilic cream SR...	267640	1
Bombastus	Anionic hydrophilic cream SR...	264751	3
Gehe	Anionic hydrophilic cream SR...	269226	1
Bombastus	Anionic hydrophilic cream SR...	267642	2
Bombastus	Anionic hydrophilic cream SR...	269227	2
Caelo	Anionic hydrophilic cream DAB		7
Bombastus	Anionic hydrophilic cream SR...	269235	1
Bombastus	Anionic hydrophilic cream SR...	269231	1
Bombastus	Anionic hydrophilic cream SR...	269236	1
Bombastus	Anionic hydrophilic cream SR...	269234	1
Bombastus	Anionic hydrophilic cream SR...	269317	1
Bombastus	Anionic hydrophilic cream SR...	271701	2
Defektur	Anionic hydrophilic cream SR...	271711	1
Noweda	Anionic hydrophilic cream SR...	271711	1
Bombastus	Anionic hydrophilic cream SR...	271837	2
Gehe	Anionic hydrophilic cream SR...	272515	3
Gehe	Anionic hydrophilic cream SR...	271838	1
Bombastus	Anionic hydrophilic cream SR...	272516	1
Bombastus	Anionic hydrophilic cream SR...	273694	2
Bombastus	Anionic hydrophilic cream SR...	273695	2
Bombastus	Anionic hydrophilic cream SR...	273693	1
Noweda	Anionic hydrophilic cream SR...	273695	1
Gehe	Anionic hydrophilic cream SR...	273694	1
Sanacorp	Anionic hydrophilic cream SR...	274376	1
Caelo	Anionic hydrophilic cream SR...	274377	2
Anzag	Anionic hydrophilic cream SR...	274377	1
Bombastus	Anionic hydrophilic cream SR...	274378	3
Bombastus	Anionic hydrophilic cream SR...	274377	1
AMH Niemann/E	Anionic hydrophilic cream SR...	1A080113	3
Apomix	Anionic hydrophilic cream wit...	6B220513	1
Apomix / Phönix	Anionic hydrophilic cream SR...	3A280114	1
Apomix	Anionic hydrophilic cream SR...	5A200212	1
Bombastus	Anionic hydrophilic cream SR...	274379	1
Apomix	Anionic hydrophilic cream wit...	7B180613	1
Caelo	Anionic hydrophilic cream SR...	8061203	1
Bombastus	Anionic hydrophilic cream SR...	80616-09	1
AMH Niemann GmbH & Co K...	Anionic hydrophilic cream SR...	7A270213	2
AMH Niemann / Phoenix	Anionic hydrophilic cream wit...	7B180613	1
apomix/GEHE/17.04.2013	Anionic hydrophilic cream SR...	8A270213	1
apomix.de	Anionic hydrophilic cream SR...	8A270213	1
Caelo	Anionic hydrophilic cream SR...	9011304	1
AMH Niemann/G	Anionic hydrophilic cream wit...	10B160712	1
Caelo	Anionic hydrophilic cream SR...	11101301	1
Bombastus	Anionic hydrophilic cream SR...	12121201	1
Pönix/AMH	Anionic hydrophilic cream SR...	11A070313	1
Phönix Gotha	Anionic hydrophilic cream SR...	122131	3

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Supplier	Substance	Batch	Spectra
Apomix	Anionic hydrophlic cream wit...	12B040912	1
Caelo	Anionic hydrophilic cream SR...	13128701	1
PKH GmbH/ Phönix	Anionic hydrophilic cream SR...	14A030413	1
apomix/E	Anionic hydrophilic cream SR...	13A190313	1
AMH Niemann/K	Anionic hydrophlic cream wit...	14B161213	1
Apomix/Alliance Healthc...	Anionic hydrophilic cream SR...	15A040413	3
Caelo	Anionic hydrophilic cream SR...	13072401	1
Caelo	Anionic hydrophilic cream SR...	15111306	1
Bombastus	Anionic hydrophilic cream SR...	15121201	1
Apomix	Anionic hydrophilic cream SR...	15A040413	1
Caelo	Anionic hydrophilic cream SR...	15011413	1
apomix/GEHE/10.07.2013	Anionic hydrophilic cream SR...	15A040413	1
Apomix	Anionic hydrophilic cream SR...	16A060611	1
PKH Halle / Phoenix	Anionic hydrophilic cream SR...	16A240413	2
apomix	Anionic hydrophilic cream SR...	16A240413	3
Apomix	Anionic hydrophilic cream SR...	17A240413	2
Caelo	Anionic hydrophilic cream SR...	18121202	1
AMH Niemann/K	Anionic hydrophlic cream wit...	17B271212	1
AMH Niemann/Anzag	Anionic hydrophilic cream SR...	17A240413	1
Caelo	Anionic hydrophilic cream SR...	20A080513	1
Bombastus	Anionic hydrophilic cream SR...	18A070513	1
Caelo	Anionic hydrophilic cream SR...	20061205	1
Apomix	Anionic hydrophilic cream SR...	18A180612	1
Caelo	Anionic hydrophilic cream SR...	22061205	1
apomix	Anionic hydrophilic cream SR...	18A180612	1
Caelo	Anionic hydrophilic cream SR...	21111202	1
Phoenix	Anionic hydrophilic cream SR...	18A260514	1
Caelo	Anionic hydrophilic cream SR...	23041307	1
Phönix Gotha	Anionic hydrophilic cream SR...	241111	1
AMH Niemann/G	Anionic hydrophilic cream SR...	18A180612	1
AMH Niemann/G	Anionic hydrophilic cream SR...	24A070812	1
ApoMix	Anionic hydrophilic cream SR...	25A210812	1
Apomix	Anionic hydrophilic cream SR...	26A220812	1
Caelo	Anionic hydrophilic cream SR...	268979	1
Caelo	Anionic hydrophilic cream SR...	25021413	1
Bombastus	Anionic hydrophilic cream SR...	271699	1
Gehe	Anionic hydrophilic cream SR...	272509	1
Bombastus	Anionic hydrophilic cream SR...	272510	1
Bombastus	Anionic hydrophilic cream SR...	272511	1
Bombastus	Anionic hydrophilic cream SR...	272514	1
Gehe	Anionic hydrophilic cream SR...	273692	1
Bombastus	Anionic hydrophilic cream SR...	274373	1
Bombastus	Anionic hydrophilic cream SR...	274381	3
Gehe	Anionic hydrophilic cream SR...	274375	1
Fiebi 23.11.12 ek:4,70	Anionic hydrophilic cream SR...	274504	2
Bombastus	Anionic hydrophilic cream SR...	274504	2
Bombastus	Anionic hydrophilic cream SR...	274505	1
Bombastus	Anionic hydrophilic cream SR...	275926	2
Bombastus	Anionic hydrophilic cream SR...	275927	3
Bombastus	Anionic hydrophilic cream SR...	276073	5
Bombastus	Anionic hydrophilic cream SR...	276074	8
Noweda	Anionic hydrophilic cream SR...	276074	1
Euro OTC	Anionic hydrophilic cream SR...	276074	1
Bombastus	Anionic hydrophilic cream SR...	276075	3
Gehe	Anionic hydrophilic cream SR...	277562	1
Bombastus	Anionic hydrophilic cream SR...	277560	2
Caelo	Anionic hydrophilic cream SR...	276077	1
Bombastus	Anionic hydrophilic cream SR...	277563	2
gehe	Anionic hydrophilic cream SR...	277563	1
Bombastus	Anionic hydrophilic cream SR...	277565	2

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Supplier	Substance	Batch	Spectra
Caelo	Anionic hydrophilic cream SR...	277565	1
Gehe	Anionic hydrophilic cream SR...	277565	1
Bombastus	Anionic hydrophilic cream SR...	277566	3
Bombastus	Anionic hydrophilic cream SR...	277569	2
Anzag ek: 5,17EUR 08.04.13	Anionic hydrophilic cream SR...	277636	3
Bombastus	Anionic hydrophilic cream SR...	277567	1
Bombastus	Anionic hydrophilic cream SR...	277568	3
Bombastus	Anionic hydrophilic cream SR...	277636	3
Bombastus	Anionic hydrophilic cream SR...	277637	5
Caelo	Anionic hydrophilic cream SR...	277636	1
Bombastus	Anionic hydrophilic cream wit...	277637	1
	Anionic hydrophilic cream SR...	277637	2
Caelo	Anionic hydrophilic cream SR...	277637	1
Sanacorp	Anionic hydrophilic cream SR...	277637	2
Bombastus	Anionic hydrophilic cream SR...	278026	2
Bombastus	Anionic hydrophilic cream SR...	279195	2
Bombastus	Anionic hydrophilic cream SR...	279199	3
Bombastus	Anionic hydrophilic cream SR...	279198	2
Bombastus	Anionic hydrophilic cream SR...	279323	1
Bombastus	Anionic hydrophilic cream SR...	279200	2
Bombastus	Anionic hydrophilic cream SR...	279325	8
Bombastus	Anionic hydrophilic cream SR...	279201	1
Bombastus	Anionic hydrophilic cream SR...	279324	3
Bombastus	Anionic hydrophilic cream SR...	279326	8
Noweda	Anionic hydrophilic cream SR...	279326	1
Apomix	Anionic hydrophilic cream SR...	27A210911	1
Apomix	Anionic hydrophilic cream SR...	27A180613	1
Bombastus	Anionic hydrophilic cream SR...	280570	2
Bombastus	Anionic hydrophilic cream SR...	280571	1
Bombastus	Anionic hydrophilic cream SR...	280574	4
Gehe	Anionic hydrophilic cream SR...	280575	1
Gehe	Anionic hydrophilic cream SR...	280574	1
Bombastus	Anionic hydrophilic cream SR...	280572	1
Bombastus	Anionic hydrophilic cream SR...	280575	1
Bombastus	Anionic hydrophilic cream SR...	280576	9
Bombastus	Anionic hydrophilic cream SR...	280741	11
Noweda	Anionic hydrophilic cream SR...	280741	2
Bombastus	Anionic hydrophilic cream SR...	281737	3
Bombastus	Anionic hydrophilic cream SR...	281739	6
Caelo	Anionic hydrophilic cream SR...	281739	2
Bombastus	Anionic hydrophilic cream SR...	281740	4
Bombastus	Anionic hydrophilic cream SR...	281742	2
Bombastus	Anionic hydrophilic cream SR...	281744	5
Bombastus	Anionic hydrophilic cream SR...	281745	1
Bombastus	Anionic hydrophilic cream SR...	281809	2
Bombastus	Anionic hydrophilic cream SR...	283282	3
Bombastus	Anionic hydrophilic cream SR...	284077	1
Alliance Healthcare/Apo...	Anionic hydrophilic cream SR...	28A250613	2
Caelo	Anionic hydrophilic cream SR...	290530	1
Pharmachem/Phönix	Anionic hydrophilic cream SR...	290413	1
Bombastus	Anionic hydrophilic cream SR...	301357	2
AMH Niemann GmbH & Co. KG	Anionic hydrophilic cream SR...	30A0207123	1
ANZAG/Apomix/30.10.2013	Anionic hydrophilic cream SR...	30A020713	2
Bombastus	Anionic hydrophilic cream SR...	299256	1
All..Healthc./Apomix	Anionic hydrophilic cream SR...	30A020713	1
Phoenix (PKH Halle)	Anionic hydrophilic cream SR...	30A021012	1
Caelo	Anionic hydrophilic cream SR...	31071301	1
Apomix	Anionic hydrophilic cream SR...	33A220713	1
Apomix	Anionic hydrophilic cream SR...	31A030713	1
Phoenix (PKH Halle)	Anionic hydrophilic cream SR...	33A151012	1

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Supplier	Substance	Batch	Spectra
AMH Niemann/E	Anionic hydrophilic cream SR...	31A091012	1
Apomix/Phoenix	Anionic hydrophilic cream SR...	33A220713	1
GEHE/apomix/01.03.2012	Anionic hydrophilic cream SR...	33A291111	1
Alliance Healthcare/Apo...	Anionic hydrophilic cream SR...	34A060813	2
AMH Niemann/K	Anionic hydrophilic cream SR...	36A270813	1
apomix	Anionic hydrophilic cream SR...	35A081112	1
Eigenherstellung	Anionic hydrophilic cream SR...	3812E-07664	1
Eigenherstellung	Anionic hydrophilic cream SR...	4012Q-07664	1
AMH Niemann/G	Anionic hydrophilic cream SR...	38A271112	1
Apomix	Anionic hydrophilic cream SR...	41A021013	1
AMH Niemann/G	Anionic hydrophilic cream SR...	44A051113	1
AMH Niemann/E	Anionic hydrophilic cream SR...	42A141013	1
Apomix	Anionic hydrophilic cream SR...	4546279	1
Apomix	Anionic hydrophilic cream SR...	44A051113	1
Bombastus	Anionic hydrophilic cream SR...	5012E-03327	1
Apomix	Anionic hydrophilic cream SR...	48A031213	1
Anzag/apomix/31.01.2014	Anionic hydrophilic cream SR...	51A171213	1
Bombastus	Anionic hydrophilic cream SR...	82440	1
Bombastus	Anionic hydrophilic cream SR...	60089211	1
Caelo	Base cream, hydrophobic DAC	4004319	1
Pharmachem	Base cream, hydrophobic DAC	110413	7
Caesar & Loretz GmbH Hi...	Base cream, hydrophobic DAC	115421302	1
Fagron	Base cream, hydrophobic DAC	13H13-T06	2
Caelo	Base cream, hydrophobic DAC	14000701	16
Caelo	Base cream, hydrophobic DAC	1400701	1
Caelo	Base cream, hydrophobic DAC	14028101	22
Phoenix	Base cream, hydrophobic DAC	14028101	1
Caelo	Base cream, hydrophobic DAC	14028102	8
Pharmachem GmbH & CoKG	Base cream, hydrophobic DAC	140318	1
Caesar & Loretz GmbH	Base cream, hydrophobic DAC	14061501	3
Phönix	Base cream, hydrophobic DAC	14061501	1
Caelo	Base cream, hydrophobic DAC	14061501	20
Euro OTC	Base cream, hydrophobic DAC	14061501	1
Pharmachen	Base cream, hydrophobic DAC	140885	1
gehe	Base cream, hydrophobic DAC	140886	2
Pharmachem/ Sanacorp	Base cream, hydrophobic DAC	140886	1
Pharmachem GmbH & CoKG	Base cream, hydrophobic DAC	140886	1
PHARMACHEM / 20	Base cream, hydrophobic DAC	140885	1
Caelo	Base cream, hydrophobic DAC	14120903	4
Gehe	Base cream, hydrophobic DAC	141317	2
Pharmachem	Base cream, hydrophobic DAC	141317	2
Pharmachem.Pößneck/Phoe...	Base cream, hydrophobic DAC	141317	1
Gehe	Base cream, hydrophobic DAC	141318	2
Pharmachem/Gehe	Base cream, hydrophobic DAC	141318	1
Pharmachem/30	Base cream, hydrophobic DAC	141317	2
Caelo	Base cream, hydrophobic DAC	14145202	3
Caelo	Base cream, hydrophobic DAC	14145301	16
AHD	Base cream, hydrophobic DAC	14145401	1
Phoenix	Base cream, hydrophobic DAC	14145401	2
Berkel AHK	Base cream, hydrophobic DAC	14145401	1
Kehr / Pharmachem	Base cream, hydrophobic DAC	141489	1
Pharmachem GmbH&Co.KG	Base cream, hydrophobic DAC	141489	1
Pharmachem/ Noweda	Base cream, hydrophobic DAC	142154	1
Pharmachem	Base cream, hydrophobic DAC	142154	3
Pharmachem/Alliance He...	Base cream, hydrophobic DAC	142154	1
Gehe	Base cream, hydrophobic DAC	142155	1
Pharmachem/Phoenix	Base cream, hydrophobic DAC	142154	2
Pharmachem	Base cream, hydrophobic DAC	142155	2
Pharmachem/Alliance Hea...	Base cream, hydrophobic DAC	142155	1
Caelo	Base cream, hydrophobic DAC	14215701	6

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Supplier	Substance	Batch	Spectra
Pharmachem	Base cream, hydrophobic DAC	143093	6
Pharmachem GmbH & CoKG	Base cream, hydrophobic DAC	143093	2
Pharmachem Pölkneck/Sana...	Base cream, hydrophobic DAC	143093	2
Pharmachen	Base cream, hydrophobic DAC	143094	1
Pharmachem/Sanacorp	Base cream, hydrophobic DAC	143094	1
Gehe	Base cream, hydrophobic DAC	143119	1
Caesar & Loretz GmbH	Base cream, hydrophobic DAC	14335501	2
Caelo	Base cream, hydrophobic DAC	14335501	10
Caelo	Base cream, hydrophobic DAC	14335502	4
Caelo	Base cream, hydrophobic DAC	14335601	5
Fagron	Base cream, hydrophobic DAC	14A06-T07-009033	3
Fagron	Base cream, hydrophobic DAC	14A06-T08-009037	3
Fagron	Base cream, hydrophobic DAC	14A06T08009038	1
Caelo	Base cream, hydrophobic DAC	15001002	8
Caelo	Base cream, hydrophobic DAC	15001001	4
Pharmachem	Base cream, hydrophobic DAC	150404	3
Caelo	Base cream, hydrophobic DAC	150405	1
Caelo	Base cream, hydrophobic DAC	15044702	4
Caelo	Base cream, hydrophobic DAC	15048701	10
Caelo	Base cream, hydrophobic DAC	15046401	7
Caesar & Loretz GmbH	Base cream, hydrophobic DAC	15048701	2
Caelo	Base cream, hydrophobic DAC	15111402	9
Caelo	Base cream, hydrophobic DAC	15111401	4
Pharmachem Pölkneck/Sana...	Base cream, hydrophobic DAC	151257	1
Pharmachem	Base cream, hydrophobic DAC	151257	4
Pharmachen	Base cream, hydrophobic DAC	151258	3
Caelo	Base cream, hydrophobic DAC	151259	3
Pharmachem	Base cream, hydrophobic DAC	151259	4
Pharmachem/Gehe	Base cream, hydrophobic DAC	151259	5
Pharmachem/ Noweda	Base cream, hydrophobic DAC	151259	1
Caelo	Base cream, hydrophobic DAC	15132502	3
Pharmachem/Sanacorp	Base cream, hydrophobic DAC	151259	2
Pharmachem/Gehe	Base cream, hydrophobic DAC	152209	1
Pharmachem/ Noweda	Base cream, hydrophobic DAC	152209	1
Pharmachen GmbH	Base cream, hydrophobic DAC	152209	1
Pharmachem Pölkneck/Sana...	Base cream, hydrophobic DAC	152210	1
Pharmachem/Sanacorp	Base cream, hydrophobic DAC	15221	1
Caelo	Base cream, hydrophobic DAC	15221202	9
Pharmachem	Base cream, hydrophobic DAC	152211	3
Pharmachem	Base cream, hydrophobic DAC	152210	2
Caelo	Base cream, hydrophobic DAC	15221301	8
Noweda	Base cream, hydrophobic DAC	15221301	4
Pharmachem/Gehe	Base cream, hydrophobic DAC	152211	1
Caesar & Loretz GmbH	Base cream, hydrophobic DAC	15221401	1
Pharmachem	Base cream, hydrophobic DAC	153625	6
Pharmachem Pölkneck/Sana...	Base cream, hydrophobic DAC	153625	1
Pharmachem Pölkneck/Sana...	Base cream, hydrophobic DAC	153626	1
Pharmachem/Gehe	Base cream, hydrophobic DAC	153625	1
Pharmachem /Phönix	Base cream, hydrophobic DAC	153626	1
Pharmachem	Base cream, hydrophobic DAC	153627	1
Caelo	Base cream, hydrophobic DAC	15421201	11
Caelo	Base cream, hydrophobic DAC	15421302	4
Caelo	Base cream, hydrophobic DAC	15421401	7
Ebert u. Jacobi 16.0...	Base cream, hydrophobic DAC	160130	1
Pharmachem	Base cream, hydrophobic DAC	160136	3
Caelo	Base cream, hydrophobic DAC	160136	1
Pharmachem/Alliance Hea...	Base cream, hydrophobic DAC	160138	1
Pharmachem Pölkneck/Sana...	Base cream, hydrophobic DAC	160137	2
Caelo	Base cream, hydrophobic DAC	16074802	9
Caelo	Base cream, hydrophobic DAC	16074901	6

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Supplier	Substance	Batch	Spectra
Caelo	Base cream, hydrophobic DAC	16074803	2
Caelo	Base cream, hydrophobic DAC	16075101	5
Phoenix	Base cream, hydrophobic DAC	16075101	2
Caelo	Base cream, hydrophobic DAC	16075201	7
Noweda	Base cream, hydrophobic DAC	16074901	2
Pharmachem/Sanacorp	Base cream, hydrophobic DAC	160814	1
Pharmachem GmbH&Co.KG	Base cream, hydrophobic DAC	160825	3
Pharmachem Pößneck/Sana. . .	Base cream, hydrophobic DAC	160826	2
Caelo	Base cream, hydrophobic DAC	1615501	1
Caelo	Base cream, hydrophobic DAC	16165501	5
Caelo	Base cream, hydrophobic DAC	16165403	6
Caelo	Base cream, hydrophobic DAC	16165502	1
Pharmachem	Base cream, hydrophobic DAC	162167	2
Pharmchem/Sanacorp	Base cream, hydrophobic DAC	162169	1
Pharmachem	Base cream, hydrophobic DAC	162169	3
Caelo	Base cream, hydrophobic DAC	16293701	1
Fagron	Base cream, hydrophobic DAC	16E03-T02-032868	1
Caelo	Base cream, hydrophobic DAC	230115/2	1
Kehr/ Pharmachem	Base cream, hydrophobic DAC	231213	2
gehe	Base cream, hydrophobic DAC	231213	3
Caelo	Base cream, hydrophobic DAC	282163	1
Bombastus	Base cream, hydrophobic DAC	286514	1
Bombastus	Base cream, hydrophobic DAC	286516	3
Caelo	Base cream, hydrophobic DAC	286516	1
Bombastus	Base cream, hydrophobic DAC	288499	3
Bombastus	Base cream, hydrophobic DAC	289718	1
Gehe/apomix/17.12.2014	Base cream, hydrophobic DAC	289719	1
Gehe	Base cream, hydrophobic DAC	289721	1
Bombastus	Base cream, hydrophobic DAC	291590	3
Bombastus	Base cream, hydrophobic DAC	293163	2
Bombastus	Base cream, hydrophobic DAC	293168	3
Caelo	Base cream, hydrophobic DAC	293163	1
Caelo	Base cream, hydrophobic DAC	294686	1
Bombastus	Base cream, hydrophobic DAC	297045	1
Bombastus	Base cream, hydrophobic DAC	300417	3
Bombastus	Base cream, hydrophobic DAC	301455	1
Bombastus	Base cream, hydrophobic DAC	303376	2
Bombastus	Base cream, hydrophobic DAC	264854	1
Pharmachem/Gehe	Base cream, hydrophobic DAC	21013	1
Gehe	Base cream, hydrophobic DAC	21013	1
Pharmachem GmbH&Co.KG	Base cream, hydrophobic DAC	21013	1
Pharmachem GmbH & CoKG	Base cream, hydrophobic DAC	21013	1
Gehe	Base cream, hydrophobic DAC	90512	1
Sanacorp/ Pharmachem	Base cream, hydrophobic DAC	90512	3
PharmaChem	Base cream, hydrophobic DAC	90512	1
Caelo	Base cream, hydrophobic DAC	11038904	1
Caelo	Base cream, hydrophobic DAC	11038802	2
Noweda	Base cream, hydrophobic DAC	110413	2
Pharmachem / Anzag	Base cream, hydrophobic DAC	110413	2
Caelo	Base cream, hydrophobic DAC	11289203	1
Caesar & Loretz GmbH, 4. . .	Base cream, hydrophobic DAC	11289203	1
Caelo	Base cream, hydrophobic DAC	11341301	2
Caelo	Base cream, hydrophobic DAC	113401301	1
Caelo	Base cream, hydrophobic DAC	11222003	1
Taoasis	Base cream, hydrophobic DAC	120214-2023	1
Fagron	Base cream, hydrophobic DAC	11L12-T05	1
Caelo	Base cream, hydrophobic DAC	11289204	1
Caelo	Base cream, hydrophobic DAC	11341402	2
Noweda	Base cream, hydrophobic DAC	11341401	1
Caelo	Base cream, hydrophobic DAC	12025002	2

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Supplier	Substance	Batch	Spectra
Noweda	Base cream, hydrophobic DAC	12025002	4
Caelo	Base cream, hydrophobic DAC	12064703	3
Caelo	Base cream, hydrophobic DAC	12064704	5
Taoasis	Base cream, hydrophobic DAC	120601-2137	1
Caelo	Base cream, hydrophobic DAC	12025003	2
Pharmachem / Anzag	Base cream, hydrophobic DAC	120712	1
Pharmachem GmbH	Base cream, hydrophobic DAC	120712	1
Pharmachem GmbH	Base cream, hydrophobic DAC	120712	2
Taoasis	Base cream, hydrophobic DAC	120719-2199	1
Caelo	Base cream, hydrophobic DAC	12064705	6
Noweda	Base cream, hydrophobic DAC	12151601	3
Taoasis	Base cream, hydrophobic DAC	121205-2299	1
Taoasis	Base cream, hydrophobic DAC	121205-2276	1
Caelo	Base cream, hydrophobic DAC	12151601	10
Caelo	Base cream, hydrophobic DAC	12151602	6
Anzag 07.05.13 ek:12,66EUR	Base cream, hydrophobic DAC	12229302	1
Caelo	Base cream, hydrophobic DAC	12229302	7
Caelo	Base cream, hydrophobic DAC	12308102	4
Gehe	Base cream, hydrophobic DAC	12308102	1
Anzag 30.10.12 ek:12,68EUR	Base cream, hydrophobic DAC	12151601	1
Caelo	Base cream, hydrophobic DAC	12308201	5
Noweda	Base cream, hydrophobic DAC	12308201	2
Fagron	Base cream, hydrophobic DAC	12J24-T01	6
Caelo	Base cream, hydrophobic DAC	12308202	2
Hirsch	Base cream, hydrophobic DAC	12J24-T01	2
Caelo	Base cream, hydrophobic DAC	13019302	6
Taoasis	Base cream, hydrophobic DAC	130124-3021	1
Sanacorp	Base cream, hydrophobic DAC	13019303	1
Noweda	Base cream, hydrophobic DAC	13019303	6
Caelo	Base cream, hydrophobic DAC	13019303	14
Taoasis	Base cream, hydrophobic DAC	130312-3053	1
Caelo	Base cream, hydrophobic DAC	13072602	5
Caelo	Base cream, hydrophobic DAC	13019304	3
calo	Base cream, hydrophobic DAC	13072602	3
Caelo	Base cream, hydrophobic DAC	13085601	11
Caelo	Base cream, hydrophobic DAC	13085602	6
Caelo	Base cream, hydrophobic DAC	13085701	23
Kehr	Base cream, hydrophobic DAC	131011	1
Gehe	Base cream, hydrophobic DAC	131011	1
Caelo	Base cream, hydrophobic DAC	13175901	20
Caelo	Base cream, hydrophobic DAC	131211	2
Gehe	Base cream, hydrophobic DAC	13175901	1
Phönix	Base cream, hydrophobic DAC	13175901	3
Caelo	Base cream, hydrophobic DAC	13175902	8
Gehe	Base cream, hydrophobic DAC	13175902	1
Caelo	Base cream, hydrophobic DAC	13275301	11
Caesar & Loretz GmbH	Base cream, hydrophobic DAC	13275302	2
Sanacorp	Base cream, hydrophobic DAC	13275302	2
Caelo	Base cream, hydrophobic DAC	13275303	4
Caelo	Base cream, hydrophobic DAC	13386401	11
Phönix	Base cream, hydrophobic DAC	13386402	2
Caesar & Loretz GmbH	Base cream, hydrophobic DAC	13386401	2
Gehe	Base cream, hydrophobic DAC	13386402	1
Caelo	Base cream, hydrophobic DAC	13386403	1
Caelo	Base cream, hydrophobic DAC	13B04-T17-001037	2
Fagron	Base cream, hydrophobic DAC	13E13-T01-003619	6
Phoenix	Base cream, hydrophobic DAC	14061501	2
Fagron	Base cream, hydrophobic DAC	13B04-T17-001037	3
Caesar & Loretz GmbH	Base cream, hydrophobic DAC	14000701	3
Fagron	Base cream, hydrophobic DAC	13H13-T06-006165	4

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Supplier	Substance	Batch	Spectra
Phönix	Base cream, hydrophobic DAC	14000701	1
Caesar&lorenz,Phoenix	Base cream, hydrophobic DAC	14335502	1
Pharmachem/Gehe	Base cream, hydrophobic DAC	230713	2
Caelo	Base cream, hydrophobic DAC	230713	3
Pharmachem GmbH	Base cream, hydrophobic DAC	240113	2
Pharmachem/Gehe	Base cream, hydrophobic DAC	240113	2
Bombastus	Base cream, hydrophobic DAC	261112	2
Pharmachem/ Sanacorp	Base cream, hydrophobic DAC	261112	2
Bombastus	Base cream, hydrophobic DAC	271092	3
Bombastus	Base cream, hydrophobic DAC	276085	1
Bombastus	Base cream, hydrophobic DAC	282163	1
Phönix Gotha	Base cream, hydrophobic DAC	276087	2
Bombastus	Base cream, hydrophobic DAC	279147	1
Sanacorp	Anionic hydrophilic cream SR...	293133	2
Bombastus	Anionic hydrophilic cream SR...	295172	1
Caelo	Base cream, hydrophobic DAC	1414501	1
Caelo	Base cream, hydrophobic DAC	15046402	3
Pharmachem Pößneck/Phoe...	Base cream, hydrophobic DAC	153627	1
Caelo	Base cream, hydrophobic DAC	16075003	3
Pharmachem/Phoenix	Base cream, hydrophobic DAC	162168	1
Bombastus	Base cream, hydrophobic DAC	298353	2
Caelo	Base cream, hydrophobic DAC	11153902	1
Caelo	Base cream, hydrophobic DAC	11222002	1
Anzag/Pharmachem	Base cream, hydrophobic DAC	120712	2
Caelo	Base cream, hydrophobic DAC	12292102	1
Gutenberg-Apotheke	Anionic hydrophilic cream SR...	285890	1
Bombastus	Anionic hydrophilic cream SR...	286974	1
Bombastus	Anionic hydrophilic cream SR...	286977	1
Bombastus	Anionic hydrophilic cream SR...	286978	1
Bombastus	Anionic hydrophilic cream SR...	288231	1
Bombastus	Anionic hydrophilic cream SR...	288228	1
Bombastus	Anionic hydrophilic cream SR...	289324	1
Bombastus	Anionic hydrophilic cream SR...	290526	1
Bombastus	Anionic hydrophilic cream SR...	290527	2
Bombastus	Anionic hydrophilic cream SR...	291522	2
Bombastus	Anionic hydrophilic cream SR...	291527	1
Bombastus	Anionic hydrophilic cream SR...	292973	1
Bombastus	Anionic hydrophilic cream SR...	283281	3
Sanacorp	Anionic hydrophilic cream SR...	283283	1
Sanacorp	Anionic hydrophilic cream SR...	283284	1
Pharmachem	Skin care ointment W/L SR	20316	1
Apomix	Skin care ointment W/L SR	16A250314	2
Pharmachem/ Sanacorp	Skin care ointment W/L SR	141015	1
Pharmachem	Skin care ointment W/L SR	90216	1
Pharmachem / Noweda	Skin care ointment W/L SR	170815	1
Pharmachem/ Noweda	Skin care ointment W/L SR	180914	1
Apomix	Skin care ointment W/L SR	17A250314	1
Apomix/ Sanacorp	Skin care ointment W/L SR (w...	15B220216	1
Apomix	Skin care ointment W/L SR	22A230414	1
Apomix	Skin care ointment W/L SR	21A230414	1
Euro OTC	Skin care ointment W/L SR	300316	1
Apomix/ Sanacorp	Skin care ointment W/L SR (w...	41B200715	1
Pharmachem/ Noweda	Skin care ointment W/L SR	260814	1
pkh gmbh	Skin care ointment W/L SR (w...	49b171014	1
Apomix	Skin care ointment W/L SR	1A080114	1
Apomix	Skin care ointment W/L SR	2A090114	1
Apomix	Skin care ointment W/L SR	9A260213	1
Apomix	Skin care ointment W/L SR	11A190214	1
Apomix	Skin care ointment W/L SR	211112	1
Pharmachem/Gehe	Skin care ointment W/L SR	100712	1

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Supplier	Substance	Batch	Spectra
Gehe	Hydrophilic cream, non-ionic...		1
Apomix	Hydrophilic cream, non-ionic...	1B070116	1
apomix/Phönix	Hydrophilic cream, non-ionic...	5A080316	3
Pharmachem GmbH&Co.KG	Hydrophilic cream, non-ionic...	90714	1
Pharmachem	Hydrophilic cream, non-ionic...	90714	5
Apomix	Hydrophilic cream, non-ionic...	5A080316	1
Apomix / 11	Hydrophilic cream, non-ionic...	10B060514	1
Sanacorp	Anionic hydrophilic cream DAB	104/AKD4	1
apomix	Hydrophilic cream, non-ionic...	3B020215	1
Fagron	Hydrophilic cream, non-ionic...	11A180416	1
Caelo	Anionic hydrophilic cream DAB	1259487	1
Apomix	Hydrophilic cream, non-ionic...	12B210514	1
Caelo	Anionic hydrophilic cream DAB	12886	1
Phönix Gotha	Hydrophilic cream, non-ionic...	12B211015	1
Caelo	Anionic hydrophilic cream DAB	13315001	7
Caelo	Anionic hydrophilic cream DAB	13314201	8
Caelo	Anionic hydrophilic cream DAB	13265602	6
Caelo	Anionic hydrophilic cream DAB	13363201	9
Caelo	Anionic hydrophilic cream DAB	1336301	1
Caelo	Anionic hydrophilic cream DAB	13346201	3
Caelo	Anionic hydrophilic cream DAB	13363601	12
Caelo	Anionic hydrophilic cream DAB	13364001	12
Caelo	Anionic hydrophilic cream DAB	13364101	4
Caelo	Anionic hydrophilic cream DAB	14016701	5
Caelo	Anionic hydrophilic cream DAB	14016901	1
Caelo	Anionic hydrophilic cream DAB	14024901	1
Phönix Gotha	Hydrophilic cream, non-ionic...	140551	4
Caelo	Anionic hydrophilic cream DAB	14062201	8
Caelo	Anionic hydrophilic cream DAB	14062101	6
Großhandel	Anionic hydrophilic cream DAB	14062101	1
Caelo	Anionic hydrophilic cream DAB	14061801	8
Caelo	Anionic hydrophilic cream DAB	14062301	7
Großhandel	Anionic hydrophilic cream DAB	14062301	1
Caelo	Anionic hydrophilic cream DAB	14062601	9
Caelo	Anionic hydrophilic cream DAB	14062701	3
Caelo	Anionic hydrophilic cream DAB	14062901	7
Caelo	Anionic hydrophilic cream DAB	14062801	4
Caelo	Anionic hydrophilic cream DAB	14068601	1
Caelo	Anionic hydrophilic cream DAB	14118101	9
Caelo	Anionic hydrophilic cream DAB	14118201	7
Caelo	Anionic hydrophilic cream DAB	14118401	8
Caelo	Anionic hydrophilic cream DAB	14118301	4
Caelo	Anionic hydrophilic cream DAB	14118501	8
Caelo	Anionic hydrophilic cream DAB	14139001	2
Caelo	Anionic hydrophilic cream DAB	14144301	4
Caelo	Anionic hydrophilic cream DAB	14144701	3
Caelo	Anionic hydrophilic cream DAB	14146301	3
Caelo	Anionic hydrophilic cream DAB	14146401	2
Phönix Gotha	Hydrophilic cream, non-ionic...	141521	2
Caelo	Anionic hydrophilic cream DAB	14185501	5
Caelo	Anionic hydrophilic cream DAB	14185701	1
Caelo	Anionic hydrophilic cream DAB	14185801	5
Caelo	Anionic hydrophilic cream DAB	14186601	6
Fagron	Anionic hydrophilic cream DAB	14186601	1
Caelo	Anionic hydrophilic cream DAB	14186702	5
Phönix Gotha	Hydrophilic cream, non-ionic...	142311	2
Caelo	Anionic hydrophilic cream DAB	14233101	6
Caelo	Anionic hydrophilic cream DAB	14233202	6
Caelo	Anionic hydrophilic cream DAB	14233401	6
Caelo	Anionic hydrophilic cream DAB	14233601	5

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Supplier	Substance	Batch	Spectra
Caelo	Anionic hydrophilic cream DAB	14263901	7
Caelo	Anionic hydrophilic cream DAB	14264001	5
Caelo	Anionic hydrophilic cream DAB	14264101	3
Caelo	Anionic hydrophilic cream DAB	14264201	7
Anzag 27.03.2015	Anionic hydrophilic cream DAB	14264301	1
Caelo	Anionic hydrophilic cream DAB	14267401	1
Caelo	Anionic hydrophilic cream DAB	14285501	3
Caelo	Anionic hydrophilic cream DAB	14285601	6
Caelo	Anionic hydrophilic cream DAB	14286101	5
Caelo	Anionic hydrophilic cream DAB	14285902	2
Caelo	Anionic hydrophilic cream DAB	14294902	1
Caelo	Anionic hydrophilic cream DAB	14286201	8
Caelo	Anionic hydrophilic cream DAB	14295001	4
Phönix Gotha	Hydrophilic cream, non-ionic...	143011	3
Caelo	Hydrophilic cream, non-ionic...	14304902	6
Henry Lamotte Oils GmbH	Anionic hydrophilic cream DAB	14341901	1
Caelo	Anionic hydrophilic cream DAB	14342201	5
Caelo	Anionic hydrophilic cream DAB	14342801	10
Caelo	Anionic hydrophilic cream DAB	14342501	3
Caelo	Anionic hydrophilic cream DAB	14342701	2
Caelo	Anionic hydrophilic cream DAB	14341501	4
AHDE 22.05.2015	Anionic hydrophilic cream DAB	14366801	5
Caelo	Anionic hydrophilic cream DAB	14366301	4
Caelo	Anionic hydrophilic cream DAB	14366801	7
Caelo	Anionic hydrophilic cream DAB	14367001	12
Phönix Gotha	Hydrophilic cream, non-ionic...	144811	5
Caelo	Anionic hydrophilic cream DAB	14367401	7
Caelo	Anionic hydrophilic cream DAB	1485401	1
Caelo	Anionic hydrophilic cream DAB	15001101	5
Caelo	Anionic hydrophilic cream DAB	15001301	6
Caelo	Anionic hydrophilic cream DAB	15001401	7
Caelo	Anionic hydrophilic cream DAB	1500141	3
Caelo	Anionic hydrophilic cream DAB	15026901	3
Caelo	Anionic hydrophilic cream DAB	15027001	11
Caelo	Anionic hydrophilic cream DAB	15027101	4
Caelo	Anionic hydrophilic cream DAB	15027002	2
Caelo	Anionic hydrophilic cream DAB	15027201	3
Caelo	Anionic hydrophilic cream DAB	15027301	3
Caelo	Anionic hydrophilic cream DAB	15034201	6
Caelo	Anionic hydrophilic cream DAB	15034301	3
Caelo	Anionic hydrophilic cream DAB	15034401	3
Caelo	Anionic hydrophilic cream DAB	15034601	5
Phönix Gotha	Hydrophilic cream, non-ionic...	150751	1
Caelo	Hydrophilic cream, non-ionic...	15037703	7
Caelo	Hydrophilic cream, non-ionic...	15039001	6
Caelo	Hydrophilic cream, non-ionic...	15155904	2
Phönix Gotha	Hydrophilic cream, non-ionic...	151711	2
Caelo	Anionic hydrophilic cream DAB	15200101	6
Caelo	Anionic hydrophilic cream DAB	15199801	2
Caelo	Hydrophilic cream, non-ionic...	15155904	1
Caelo	Anionic hydrophilic cream DAB	15200201	3
Caelo	Hydrophilic cream, non-ionic...	15210303	5
Caelo	Anionic hydrophilic cream DAB	15258901	1
Caelo	Anionic hydrophilic cream DAB	15266901	2
Caelo	Anionic hydrophilic cream DAB	15259101	4
Caelo	Anionic hydrophilic cream DAB	15259001	6
Caelo	Anionic hydrophilic cream DAB	15267101	2
Caelo	Anionic hydrophilic cream DAB	15267301	5
Caelo	Anionic hydrophilic cream DAB	15267201	5
Caelo	Anionic hydrophilic cream DAB	15267601	1

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Supplier	Substance	Batch	Spectra
phoenix/noveda	Anionic hydrophilic cream DAB	15267501	1
Caelo	Anionic hydrophilic cream DAB	15267801	6
Caelo	Anionic hydrophilic cream DAB	15267501	1
Phönix Gotha	Hydrophilic cream, non-ionic...	153041	4
Caelo	Anionic hydrophilic cream DAB	15315701	4
Caelo	Anionic hydrophilic cream DAB	15315801	1
Caelo	Anionic hydrophilic cream DAB	15315901	3
Caelo	Anionic hydrophilic cream DAB	15319301	5
Caelo	Hydrophilic cream, non-ionic...	15325702	2
Caelo	Hydrophilic cream, non-ionic...	15325801	6
Caelo	Anionic hydrophilic cream DAB	15352901	3
Caelo	Anionic hydrophilic cream DAB	15353201	2
Caelo	Anionic hydrophilic cream DAB	15397201	4
Phönix Gotha	Hydrophilic cream, non-ionic...	153621	1
Caelo	Anionic hydrophilic cream DAB	15397301	6
LEYH PHARMA / Phönix Le...	Hydrophilic cream, non-ionic...	153621	1
Caelo	Anionic hydrophilic cream DAB	15396801	2
Caesar&Loretz GmbH	Anionic hydrophilic cream DAB	15357401	1
Caelo	Anionic hydrophilic cream DAB	15400401	3
Caelo	Anionic hydrophilic cream DAB	15400701	4
Caelo	Anionic hydrophilic cream DAB	154009	1
Caelo	Anionic hydrophilic cream DAB	15400801	1
Caelo	Anionic hydrophilic cream DAB	15401001	2
Caelo	Anionic hydrophilic cream DAB	15401101	3
Caelo	Anionic hydrophilic cream DAB	15401401	3
Caelo	Anionic hydrophilic cream DAB	1541702	1
Caelo	Anionic hydrophilic cream DAB	15428102	2
Caelo	Anionic hydrophilic cream DAB	15428401	3
Caelo	Anionic hydrophilic cream DAB	15431701	3
Caelo	Anionic hydrophilic cream DAB	15432001	5
Caelo	Anionic hydrophilic cream DAB	15432101	6
Noweda	Anionic hydrophilic cream DAB	15428401	1
Leyh Pharma / Alliance ...	Hydrophilic cream, non-ionic...	155221	1
LEYH PHARMA / Phönix Le...	Hydrophilic cream, non-ionic...	155221	1
apomix/Holdermann	Hydrophilic cream, non-ionic...	15B290615	1
Caelo	Anionic hydrophilic cream DAB	16047101	1
Caelo	Anionic hydrophilic cream DAB	16046601	1
Caelo	Hydrophilic cream, non-ionic...	16054101	2
Leyh Pharma/Anzag	Hydrophilic cream, non-ionic...	160651	1
Caelo	Anionic hydrophilic cream DAB	16103201	1
Caelo	Hydrophilic cream, non-ionic...	16114102	2
Caelo	Hydrophilic cream, non-ionic...	16257902	1
Caelo	Anionic hydrophilic cream DAB	16259401	1
apomix	Hydrophilic cream, non-ionic...	17A100315	1
Gehe	Hydrophilic cream, non-ionic...	17B120814	1
Apomix / Sanacorp	Hydrophilic cream, non-ionic...	17B040815	3
Caelo	Anionic hydrophilic cream DAB	1814E2540	1
Apomix	Hydrophilic cream, non-ionic...	18B270916	2
Bombastus	Hydrophilic cream, non-ionic...	201015	3
Bombastus	Anionic hydrophilic cream DAB	280291	1
Apomix / Noweda	Hydrophilic cream, non-ionic...	23B101115	1
Pharmachem	Hydrophilic cream, non-ionic...	220713	3
Bombastus	Anionic hydrophilic cream DAB	277463	1
Caelo	Anionic hydrophilic cream DAB	281999	1
Bombastus	Anionic hydrophilic cream DAB	282109	1
Bombastus	Anionic hydrophilic cream DAB	282114	4
Bombastus	Anionic hydrophilic cream DAB	282110	4
Raben-Apotheke Mildena	Anionic hydrophilic cream DAB	283410	1
Bombastus	Anionic hydrophilic cream DAB	283413	2
Bombastus	Anionic hydrophilic cream DAB	283411	2

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Supplier	Substance	Batch	Spectra
Bombastus	Anionic hydrophilic cream DAB	283474	1
Bomba	Anionic hydrophilic cream DAB	283478	1
Bombastus	Anionic hydrophilic cream DAB	283482	1
Bombastus	Hydrophilic cream, non-ionic...	284899	4
Bombastus	Anionic hydrophilic cream DAB	285592	1
Bombastus	Anionic hydrophilic cream DAB	285594	2
Bombastus	Anionic hydrophilic cream DAB	285591	1
Bombastus	Anionic hydrophilic cream DAB	285595	1
Bombastus	Anionic hydrophilic cream DAB	285596	1
Bombastus	Anionic hydrophilic cream DAB	285597	1
Bombastus	Hydrophilic cream, non-ionic...	286326	7
Bombastus	Anionic hydrophilic cream DAB	286495	1
Bombastus	Anionic hydrophilic cream DAB	286498	1
Bombastus	Anionic hydrophilic cream DAB	286502	2
Bombastus	Anionic hydrophilic cream DAB	286505	2
Bombastus	Anionic hydrophilic cream DAB	287433	1
Bombastus	Anionic hydrophilic cream DAB	287432	2
Bombastus	Anionic hydrophilic cream DAB	287557	3
Bombastus	Anionic hydrophilic cream DAB	287436	2
Bombastus	Anionic hydrophilic cream DAB	287559	1
Bombastus	Anionic hydrophilic cream DAB	287562	3
Caelo	Anionic hydrophilic cream DAB	287562	1
Bombastus	Anionic hydrophilic cream DAB	287564	2
Bombastus	Anionic hydrophilic cream DAB	287563	1
Bombastus	Anionic hydrophilic cream DAB	287565	1
Bombastus	Hydrophilic cream, non-ionic...	287761	1
Bombastus	Hydrophilic cream, non-ionic...	287763	2
Phönix	Anionic hydrophilic cream DAB	288572	1
Bombastus	Anionic hydrophilic cream DAB	288574	2
Bombastus	Anionic hydrophilic cream DAB	288653	1
Bombastus	Anionic hydrophilic cream DAB	288652	1
Bombastus	Anionic hydrophilic cream DAB	288655	2
Euro OTC	Anionic hydrophilic cream DAB	288658	1
Bombastus	Anionic hydrophilic cream DAB	288721	2
Bombastus	Anionic hydrophilic cream DAB	288658	2
Bombastus	Anionic hydrophilic cream DAB	288657	1
Bombastus	Anionic hydrophilic cream DAB	288659	3
Caelo	Hydrophilic cream, non-ionic...	28882	1
Bombastus	Anionic hydrophilic cream DAB	290144	1
Caelo	Hydrophilic cream, non-ionic...	289942	1
Bombastus	Anionic hydrophilic cream DAB	290145	2
Rabenapotheke	Anionic hydrophilic cream DAB	290146	1
Bombastus	Anionic hydrophilic cream DAB	290150	1
Bombastus	Anionic hydrophilic cream DAB	290146	4
Bombastus	Hydrophilic cream, non-ionic...	291384	1
Bombastus	Anionic hydrophilic cream DAB	291650	1
Bombastus	Anionic hydrophilic cream DAB	291656	3
Bobmastus	Anionic hydrophilic cream DAB	291657	1
Bombastus	Anionic hydrophilic cream DAB	291658	2
Bombastus	Anionic hydrophilic cream DAB	291659	1
Bombastus	Anionic hydrophilic cream DAB	291822	2
Bombastus	Anionic hydrophilic cream DAB	291732	2
Bombastus	Anionic hydrophilic cream DAB	291824	4
Bombastus	Anionic hydrophilic cream DAB	291823	2
Bombastus	Hydrophilic cream, non-ionic...	292804	3
Bombastus	Hydrophilic cream, non-ionic...	292807	2
Bombastus	Hydrophilic cream, non-ionic...	292814	6
Bombastus	Hydrophilic cream, non-ionic...	292970	1
Bombastus	Anionic hydrophilic cream DAB	293359	1
Phoenix Goettin	Anionic hydrophilic cream DAB	293439	1

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Supplier	Substance	Batch	Spectra
Bombastus	Anionic hydrophilic cream DAB	293357	1
Bombastus	Anionic hydrophilic cream DAB	293440	4
Bombastus	Anionic hydrophilic cream DAB	293437	2
Bombastus	Anionic hydrophilic cream DAB	293441	4
Bombastus	Anionic hydrophilic cream DAB	293445	1
Bombastus	Anionic hydrophilic cream DAB	293447	2
Bombastus	Anionic hydrophilic cream DAB	293448	3
Bombastus	Hydrophilic cream, non-ionic...	294407	2
Bombastus	Hydrophilic cream, non-ionic...	294406	3
Bombastus	Anionic hydrophilic cream DAB	294546	1
Bombastus	Anionic hydrophilic cream DAB	294641	1
Bombastus	Anionic hydrophilic cream DAB	294647	2
Bombastus	Anionic hydrophilic cream DAB	294547	1
Bombastus	Anionic hydrophilic cream DAB	294649	3
Bombastus	Anionic hydrophilic cream DAB	294648	1
Bombastus	Anionic hydrophilic cream DAB	294650	3
Bombastus	Anionic hydrophilic cream DAB	295396	1
Caelo	Anionic hydrophilic cream DAB	295400	1
Bombastus	Anionic hydrophilic cream DAB	295400	1
Bombastus	Anionic hydrophilic cream DAB	295516	4
Bombastus	Anionic hydrophilic cream DAB	295403	1
Bombastus	Anionic hydrophilic cream DAB	295518	5
Bombastus	Anionic hydrophilic cream DAB	295517	1
Bombastus	Hydrophilic cream, non-ionic...	295652	2
Bombastus	Anionic hydrophilic cream DAB	296703	4
Bombastus	Anionic hydrophilic cream DAB	296708	3
Bombastus	Anionic hydrophilic cream DAB	296706	1
Bombastus	Anionic hydrophilic cream DAB	296784	1
Bombastus	Anionic hydrophilic cream DAB	296783	2
Bombastus	Anionic hydrophilic cream DAB	296787	2
Bombastus	Hydrophilic cream, non-ionic...	297302	1
Bombastus	Hydrophilic cream, non-ionic...	297298	1
Bombastus	Hydrophilic cream, non-ionic...	297305	1
Fagron	Hydrophilic cream, non-ionic...	297372	1
Bombastus	Anionic hydrophilic cream DAB	297668	2
Bombastus	Anionic hydrophilic cream DAB	297676	1
Bombastus	Anionic hydrophilic cream DAB	297677	1
Bombastus	Anionic hydrophilic cream DAB	297675	2
Bombastus	Anionic hydrophilic cream DAB	297669	1
Bombastus	Anionic hydrophilic cream DAB	297679	2
Bombastus	Hydrophilic cream, non-ionic...	297911	1
Bombastus	Anionic hydrophilic cream DAB	300356	1
Bombastus	Anionic hydrophilic cream DAB	300355	1
Bombastus	Anionic hydrophilic cream DAB	300349	1
Bombastus	Hydrophilic cream, non-ionic...	300761	1
Bombastus	Hydrophilic cream, non-ionic...	300763	1
Bombastus	Hydrophilic cream, non-ionic...	300766	1
Bombastus	Hydrophilic cream, non-ionic...	301624	1
Bombastus	Hydrophilic cream, non-ionic...	302690	3
APOMIX/AHD	Hydrophilic cream, non-ionic...	35A130514	1
Caelo	Hydrophilic cream, non-ionic...	36A140514	1
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	47A2801015	1
Bombastus	Hydrophilic cream, non-ionic...	60089512	1
Bombastus	Hydrophilic cream, non-ionic...	99320	1
Bombastus	Hydrophilic cream, non-ionic...	268347	1
Bombastus	Hydrophilic cream, non-ionic...	269714	2
Gehe	Hydrophilic cream, non-ionic...	271518	1
Bombastus	Hydrophilic cream, non-ionic...	271522	2
Bombastus	Hydrophilic cream, non-ionic...	273130	4
Bombastus	Hydrophilic cream, non-ionic...	274103	2

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Supplier	Substance	Batch	Spectra
Bombastus	Hydrophilic cream, non-ionic...	272492	2
Bombastus	Hydrophilic cream, non-ionic...	274219	2
Bombastus	Hydrophilic cream, non-ionic...	274211	4
Bombastus	Hydrophilic cream, non-ionic...	273134	2
GEHE/apomix/22.05.2012	Hydrophilic cream, non-ionic...	3A130212	1
Bombastus	Hydrophilic cream, non-ionic...	274223	3
Pharmachem GmbH	Hydrophilic cream, non-ionic...	50912	1
Phönix Gotha	Hydrophilic cream, non-ionic...	4B070213	1
Noweda	Hydrophilic cream, non-ionic...	11A260312	1
Gehe	Hydrophilic cream, non-ionic...	121431	1
Phönix Gotha	Hydrophilic cream, non-ionic...	122841	4
Leyh Pharma	Hydrophilic cream, non-ionic...	122841	1
Phönix Gotha	Hydrophilic cream, non-ionic...	124511	5
Phönix	Hydrophilic cream, non-ionic...	124511	1
Leyh Pharma	Hydrophilic cream, non-ionic...	130651	2
Phönix Gotha	Hydrophilic cream, non-ionic...	131451	2
Phönix Gotha	Hydrophilic cream, non-ionic...	133121	3
Phönix Gotha	Hydrophilic cream, non-ionic...	134841	2
Fagron	Hydrophilic cream, non-ionic...	13K12-M05	1
Gehe	Hydrophilic cream, non-ionic...	14B090713	1
Fagron	Hydrophilic cream, non-ionic...	13K12-M04	1
Apomix	Hydrophilic cream, non-ionic...	16A300512	2
GEHE/apomix/13.07.2012	Hydrophilic cream, non-ionic...	13A230412	1
Apomix	Hydrophilic cream, non-ionic...	18A070612	1
Pharmachem GmbH	Hydrophilic cream, non-ionic...	220713	2
Bombastus	Hydrophilic cream, non-ionic...	277637	1
Caelo	Hydrophilic cream, non-ionic...	274223	1
Bombastus	Hydrophilic cream, non-ionic...	277873	4
Bombastus	Hydrophilic cream, non-ionic...	277878	10
Bombastus	Hydrophilic cream, non-ionic...	276252	6
Caelo	Hydrophilic cream, non-ionic...	276596	1
Bombastus	Hydrophilic cream, non-ionic...	277879	1
Bombastus	Hydrophilic cream, non-ionic...	279661	8
Apomix	Hydrophilic cream, non-ionic...	27B221012	1
Caelo	Hydrophilic cream, non-ionic...	280988	1
Gehe	Hydrophilic cream, non-ionic...	282214	1
gehe	Hydrophilic cream, non-ionic...	282211	1
Bombastus	Hydrophilic cream, non-ionic...	283637	1
Bombastus	Hydrophilic cream, non-ionic...	2886797	1
Bombastus	Hydrophilic cream, non-ionic...	283692	2
Bombastus	Hydrophilic cream, non-ionic...	291385	2
Apomix	Hydrophilic cream, non-ionic...	39A131112	1
Apomix / Phönix	Hydrophilic cream, non-ionic...	32A090713	1
Fagron	Hydrophilic cream, non-ionic...	4A220113	1
Caelo	Anionic hydrophilic cream DAB	2569516	1
Bombastus	Anionic hydrophilic cream DAB	262774	1
Bombastus	Anionic hydrophilic cream SR...	264643	1
Bombastus	Anionic hydrophilic cream DAB	264833	1
Gehe	Anionic hydrophilic cream SR...	267647	1
Bombastus	Anionic hydrophilic cream DAB	267616	1
Klenk	Anionic hydrophilic cream DAB	266259	1
Klenk	Anionic hydrophilic cream DAB	264833	1
Bombastus	Anionic hydrophilic cream SR...	264644	1
Bombastus	Anionic hydrophilic cream DAB	267442	1
Gehe	Anionic hydrophilic cream SR...	269235	1
Bombastus	Anionic hydrophilic cream DAB	269444	1
Bombastus	Anionic hydrophilic cream DAB	269513	2
Bombastus	Anionic hydrophilic cream DAB	269518	1
Bombastus	Anionic hydrophilic cream DAB	270804	1
Bombastus	Anionic hydrophilic cream DAB	269517	1

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Supplier	Substance	Batch	Spectra
Bombastus	Anionic hydrophilic cream DAB	270824	2
Bombastus	Anionic hydrophilic cream DAB	270946	1
Gehe	Anionic hydrophilic cream DAB	270949	1
Bombastus	Anionic hydrophilic cream DAB	271008	2
Gehe	Anionic hydrophilic cream DAB	271010	1
Bombastus	Anionic hydrophilic cream DAB	270950	1
Bomastus	Anionic hydrophilic cream DAB	273404	1
DAB	Anionic hydrophilic cream DAB	270951	1
Bombastus	Anionic hydrophilic cream DAB	271011	1
Bombastus	Anionic hydrophilic cream SR. . .	271710	2
Bombastus	Anionic hydrophilic cream DAB	273407	1
Bombastus	Anionic hydrophilic cream SR. . .	271702	1
Bombastus	Anionic hydrophilic cream DAB	273536	1
Bombastus	Anionic hydrophilic cream DAB	273532	1
Caelo	Anionic hydrophilic cream DAB	1061302	1
Sanacorp	Anionic hydrophilic cream SR. . .	273693	1
Bombastus	Anionic hydrophilic cream DAB	273534	1
Caelo	Anionic hydrophilic cream DAB	3061302	1
Caelo	Anionic hydrophilic cream DAB	204312540	1
Caelo	Anionic hydrophilic cream DAB	1119720	1
Caelo	Anionic hydrophilic cream DAB	413I-02540	1
Caelo	Anionic hydrophilic cream DAB	4131I-02540	1
GEHE/AMH/22.05.2012	Anionic hydrophilic cream SR. . .	5A200212	1
Caelo	Anionic hydrophilic cream DAB	6121304	1
Caelo	Anionic hydrophilic cream SR. . .	1101212540	1
Caelo	Anionic hydrophilic cream DAB	11180201	1
Caelo	Anionic hydrophilic cream DAB	1119387	1
Caelo	Anionic hydrophilic cream DAB	11120201	1
Caelo	Anionic hydrophilic cream DAB	11229001	2
Noweda	Anionic hydrophilic cream DAB	11229001	2
Caelo	Anionic hydrophilic cream DAB	11229101	1
Caelo	Anionic hydrophilic cream DAB	11229201	1
Caesar & Loretz GmbH 40. . .	Anionic hydrophilic cream DAB	11253201	1
Caelo	Anionic hydrophilic cream DAB	11253401	1
Caelo	Anionic hydrophilic cream DAB	11258201	2
Caelo	Anionic hydrophilic cream DAB	11253501	1
Caesar & Loretz GmbH, 4. . .	Anionic hydrophilic cream DAB	11311101	3
Caelo	Anionic hydrophilic cream DAB	11311101	2
Caelo	Anionic hydrophilic cream DAB	11258301	1
Gehe	Anionic hydrophilic cream DAB	11311202	1
Caelo	Anionic hydrophilic cream DAB	11311501	1
Caelo	Anionic hydrophilic cream DAB	11320901	1
Caelo	Anionic hydrophilic cream DAB	11321101	1
Caesar&lorenz,Phoenix	Anionic hydrophilic cream DAB	11320801	1
Caelo	Anionic hydrophilic cream DAB	11326701	3
Caesar & Loretz GmbH D-. . .	Anionic hydrophilic cream DAB	11326701	1
Caelo	Anionic hydrophilic cream DAB	11331501	2
Caelo	Anionic hydrophilic cream DAB	11331601	1
Caelo	Anionic hydrophilic cream DAB	11332101	1
Caelo	Anionic hydrophilic cream DAB	11332001	1
Caelo	Anionic hydrophilic cream DAB	11332401	1
Kehr	Anionic hydrophilic cream DAB	11332401	1
Caelo	Anionic hydrophilic cream DAB	11332501	1
Caelo	Anionic hydrophilic cream DAB	113332301	1
Caelo	Anionic hydrophilic cream DAB	12010201	1
Caesar&lorenz,Phoenix	Anionic hydrophilic cream DAB	12010501	1
Caelo	Anionic hydrophilic cream DAB	12010801	2
Caelo	Anionic hydrophilic cream DAB	12010901	1
Caelo	Anionic hydrophilic cream DAB	12012101	1
Phoenix	Anionic hydrophilic cream DAB	12011001	1

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Supplier	Substance	Batch	Spectra
Gehe	Anionic hydrophilic cream DAB	12026001	1
Caelo	Anionic hydrophilic cream DAB	12081301	1
Caelo	Anionic hydrophilic cream DAB	12011302	2
Caelo	Anionic hydrophilic cream DAB	12012201	1
Caelo	Anionic hydrophilic cream DAB	12083702	1
Noweda	Anionic hydrophilic cream DAB	12098801	1
Noweda	Anionic hydrophilic cream DAB	12010901	1
Caelo	Anionic hydrophilic cream DAB	12083802	1
Caelo	Anionic hydrophilic cream DAB	12098801	1
Caelo	Anionic hydrophilic cream DAB	12099001	2
Kehr	Anionic hydrophilic cream DAB	12098901	1
Caelo	Anionic hydrophilic cream DAB	12099201	3
Caelo	Anionic hydrophilic cream DAB	12099101	1
Caelo	Anionic hydrophilic cream DAB	12099301	1
Caelo	Anionic hydrophilic cream DAB	12099501	1
Noweda	Anionic hydrophilic cream DAB	12099901	2
Caelo	Anionic hydrophilic cream DAB	12100201	1
DAB 2008	Anionic hydrophilic cream DAB	12099901	1
Caelo	Anionic hydrophilic cream DAB	12100401	3
Noweda	Anionic hydrophilic cream DAB	12100401	1
Caelo	Anionic hydrophilic cream DAB	12100501	2
Caelo	Anionic hydrophilic cream DAB	12100601	5
Noweda	Anionic hydrophilic cream DAB	12100801	4
Caelo	Anionic hydrophilic cream DAB	12100701	3
Caelo	Anionic hydrophilic cream DAB	12101201	1
Noweda	Anionic hydrophilic cream DAB	12101302	5
Caelo	Anionic hydrophilic cream DAB	12100901	6
Caelo	Anionic hydrophilic cream DAB	12128502	4
Phönix Gotha	Anionic hydrophilic cream SR. ...	121431	2
Caelo	Anionic hydrophilic cream DAB	12187701	2
Caelo	Anionic hydrophilic cream DAB	12187901	8
Caelo	Anionic hydrophilic cream DAB	12195201	8
Caesar & Loretz GmbH, 4...	Anionic hydrophilic cream DAB	12195201	2
Caelo	Anionic hydrophilic cream DAB	12195401	4
Caelo	Anionic hydrophilic cream DAB	12195601	7
Caelo	Anionic hydrophilic cream DAB	12195501	2
Caelo	Anionic hydrophilic cream DAB	12204301	3
Caelo	Anionic hydrophilic cream DAB	12204501	2
Caelo	Anionic hydrophilic cream DAB	12218301	2
Großhandel	Anionic hydrophilic cream DAB	12204501	1
Anzag,23.10.2012	Anionic hydrophilic cream DAB	12209101	1
Caelo	Anionic hydrophilic cream DAB	12204601	1
Caelo	Anionic hydrophilic cream DAB	12218401	2
Caelo	Anionic hydrophilic cream DAB	12218501	2
Caelo	Anionic hydrophilic cream DAB	12218601	2
Caelo	Anionic hydrophilic cream DAB	12245601	1
Caelo	Anionic hydrophilic cream DAB	12245401	4
Caelo	Anionic hydrophilic cream DAB	12245501	1
Caelo	Anionic hydrophilic cream DAB	12264601	1
Sanacorp	Anionic hydrophilic cream DAB	12245701	1
Caesar & Loretz GmbH, 4...	Anionic hydrophilic cream DAB	12264501	1
Caelo	Anionic hydrophilic cream DAB	12245701	3
Caelo	Anionic hydrophilic cream DAB	12264801	3
Noweda	Anionic hydrophilic cream DAB	12264901	1
Caelo	Anionic hydrophilic cream DAB	12265201	6
Caelo	Anionic hydrophilic cream DAB	12265601	1
Caelo	Anionic hydrophilic cream DAB	12265301	4
Caelo	Anionic hydrophilic cream DAB	12265701	4
Noweda	Anionic hydrophilic cream DAB	12265701	1
Caelo	Anionic hydrophilic cream DAB	12266101	5

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Supplier	Substance	Batch	Spectra
Caelo	Anionic hydrophilic cream DAB	12265401	3
Caelo	Anionic hydrophilic cream DAB	12265501	4
Anzag 25.01.2013	Anionic hydrophilic cream DAB	12266101	1
Caesar & Loretz GmbH, 4...	Anionic hydrophilic cream DAB	12313202	2
Caelo	Anionic hydrophilic cream DAB	12265801	2
Caelo	Anionic hydrophilic cream DAB	12266201	3
Caelo	Anionic hydrophilic cream DAB	12313202	9
Noweda	Anionic hydrophilic cream DAB	12313202	1
Phoenix	Anionic hydrophilic cream DAB	12313301	1
Caelo	Anionic hydrophilic cream DAB	12313601	6
Caelo	Anionic hydrophilic cream DAB	12313701	8
Caelo	Anionic hydrophilic cream DAB	12313901	10
Caelo	Anionic hydrophilic cream DAB	12314001	1
Caelo	Anionic hydrophilic cream DAB	12314101	9
Anzag	Anionic hydrophilic cream DAB	12314101	1
GEHE	Anionic hydrophilic cream DAB	12314101	1
Caesar&lorenz,Phoenix	Anionic hydrophilic cream DAB	12314201	1
Caelo	Anionic hydrophilic cream DAB	12314301	5
Caelo	Anionic hydrophilic cream DAB	12314401	8
Caelo	Anionic hydrophilic cream DAB	12314701	8
Noweda	Anionic hydrophilic cream DAB	12314601	1
AHD,15.04.2013	Anionic hydrophilic cream DAB	12314701	1
Caelo	Anionic hydrophilic cream DAB	12314601	9
Hirsch	Anionic hydrophilic cream DAB	12314701	1
Caelo	Anionic hydrophilic cream DAB	12314801	8
Noweda	Anionic hydrophilic cream DAB	12314801	1
Caelo	Anionic hydrophilic cream DAB	12314901	5
Caelo	Anionic hydrophilic cream DAB	12316001	1
Noweda	Anionic hydrophilic cream DAB	13002705	1
Caelo	Anionic hydrophilic cream DAB	1303312540	1
Caelo	Anionic hydrophilic cream DAB	13035901	1
Caelo	Anionic hydrophilic cream DAB	13036001	4
Caelo	Anionic hydrophilic cream DAB	13038301	7
AHC 28.05.13 EK2,95	Anionic hydrophilic cream DAB	13036301	1
Caelo	Anionic hydrophilic cream DAB	13036301	8
Caelo	Anionic hydrophilic cream DAB	13068504	1
Caelo	Anionic hydrophilic cream DAB	13070301	6
Caelo	Anionic hydrophilic cream DAB	13070502	4
Noweda	Anionic hydrophilic cream DAB	13070301	1
Caelo	Anionic hydrophilic cream DAB	13070601	6
Caelo	Anionic hydrophilic cream DAB	13070401	1
Caelo	Anionic hydrophilic cream SR...	13071202	1
Caelo	Anionic hydrophilic cream DAB	13072501	3
Caelo	Anionic hydrophilic cream DAB	13128601	7
Caelo	Anionic hydrophilic cream DAB	13128701	9
Caelo	Anionic hydrophilic cream DAB	13154001	1
Caelo	Anionic hydrophilic cream DAB	1313314401	1
Caelo	Anionic hydrophilic cream DAB	13154101	4
Phönix	Anionic hydrophilic cream DAB	13164901	1
Noweda	Anionic hydrophilic cream DAB	13154301	1
Caelo	Anionic hydrophilic cream DAB	13154201	2
Caelo	Anionic hydrophilic cream DAB	13164901	4
Caelo	Anionic hydrophilic cream DAB	13154202	2
Caelo	Anionic hydrophilic cream DAB	13165001	9
Caelo	Anionic hydrophilic cream DAB	13165101	3
Caelo	Anionic hydrophilic cream DAB	13165601	2
Caelo	Anionic hydrophilic cream DAB	13165701	6
Caelo	Anionic hydrophilic cream DAB	13165901	6
Caelo	Anionic hydrophilic cream DAB	13165801	8
Caelo	Anionic hydrophilic cream DAB	13166001	4

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Supplier	Substance	Batch	Spectra
Caelo	Anionic hydrophilic cream DAB	13167501	8
Sanacorp	Anionic hydrophilic cream DAB	13167501	1
Caelo	Anionic hydrophilic cream DAB	13167601	2
Caelo	Anionic hydrophilic cream DAB	13167901	1
Caelo	Anionic hydrophilic cream DAB	1316801	1
Caelo	Anionic hydrophilic cream DAB	13168101	1
Caelo	Anionic hydrophilic cream DAB	13168401	9
Caelo	Anionic hydrophilic cream DAB	13168601	13
Caelo	Anionic hydrophilic cream DAB	13168801	3
Großhandel	Anionic hydrophilic cream DAB	13168801	1
Caelo	Anionic hydrophilic cream DAB	13168901	8
Caelo	Anionic hydrophilic cream DAB	13169001	10
Caelo	Anionic hydrophilic cream DAB	13265301	8
Caelo	Anionic hydrophilic cream DAB	13169301	6
Caelo	Anionic hydrophilic cream DAB	13265401	5
Caelo	Anionic hydrophilic cream DAB	13275601	2
Caelo	Anionic hydrophilic cream DAB	13270701	4
Caelo	Anionic hydrophilic cream DAB	13271101	4
Caelo	Anionic hydrophilic cream DAB	13280101	18
Caelo	Anionic hydrophilic cream DAB	13277401	9
Caelo	Anionic hydrophilic cream DAB	13277501	4
Caelo	Anionic hydrophilic cream DAB	13280201	9
Caelo	Anionic hydrophilic cream DAB	13313001	3
Caelo	Anionic hydrophilic cream DAB	13312801	5
Caelo	Anionic hydrophilic cream DAB	13313101	4
Caelo	Anionic hydrophilic cream DAB	13313201	8
Caelo	Anionic hydrophilic cream DAB	13313301	3
Caelo	Anionic hydrophilic cream DAB	13313901	9
Caelo	Anionic hydrophilic cream DAB	13313501	5
Phoenix 09.01.2014	Anionic hydrophilic cream DAB	13313501	1
Caelo	Anionic hydrophilic cream DAB	13313601	5
Caelo	Anionic hydrophilic cream DAB	13313701	6
Caelo	Anionic hydrophilic cream DAB	13314401	10
Caelo	Anionic hydrophilic cream DAB	13314001	5
Caelo	Anionic hydrophilic cream DAB	1331401	1
Caelo	Anionic hydrophilic cream DAB	13314801	2
Caesar&lorenz,Phoenix	Anionic hydrophilic cream DAB	13364301	1
Caelo	Anionic hydrophilic cream DAB	14062401	4
Caesar & Loretz GmbH	Anionic hydrophilic cream DAB	14016901	2
Caelo	Anionic hydrophilic cream DAB	13364401	5
Caelo	Anionic hydrophilic cream DAB	13364301	8
Caelo	Anionic hydrophilic cream DAB	15200601	4
Caelo	Anionic hydrophilic cream DAB	15011301	1
Caelo	Anionic hydrophilic cream DAB	1913Q-02540	1
Pharmachem	Anionic hydrophilic cream SR...	170412	2
GEHE/apomix/05.07.2012	Anionic hydrophilic cream SR...	16A050612	1
Caelo	Anionic hydrophilic cream SR...	1603212540	1
Caelo	Anionic hydrophilic cream DAB	2112212540	1
Caelo	Anionic hydrophilic cream DAB	1913R-02540	1
Caelo	Anionic hydrophilic cream DAB	2405212540	1
Caelo	Anionic hydrophilic cream DAB	2103312540	1
Caelo	Anionic hydrophilic cream DAB	2704212540	1
Phönix	Anionic hydrophilic cream DAB	270703	1
Bombastus	Anionic hydrophilic cream DAB	270704	1
Phoenix	Anionic hydrophilic cream DAB	270705	1
Caelo	Anionic hydrophilic cream DAB	27091305	1
Bombastus	Anionic hydrophilic cream DAB	270706	1
Bombastus	Anionic hydrophilic cream DAB	273401	1
Bombastus	Anionic hydrophilic cream DAB	274593	2
Bombastus	Anionic hydrophilic cream DAB	274595	2

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Supplier	Substance	Batch	Spectra
Gehe/ 28.12.12 Bambastus	Anionic hydrophilic cream DAB	274594	1
Bombastus	Anionic hydrophilic cream DAB	274554	1
Bombastus	Anionic hydrophilic cream DAB	274596	1
Bombastus	Anionic hydrophilic cream DAB	274695	2
Noweda	Anionic hydrophilic cream DAB	274697	1
Bombastus	Anionic hydrophilic cream DAB	274697	2
Bombastus	Anionic hydrophilic cream DAB	274695/273533	1
Bombastus	Anionic hydrophilic cream DAB	274765	2
Bombastus	Anionic hydrophilic cream DAB	274766	2
Bombastus	Anionic hydrophilic cream DAB	276315	2
Bombastus	Anionic hydrophilic cream DAB	276318	1
Bombastus	Anionic hydrophilic cream DAB	276320	2
Bombastus	Anionic hydrophilic cream DAB	277295	1
Caelo	Anionic hydrophilic cream DAB	276321	1
Bombastus	Anionic hydrophilic cream DAB	277293	5
Bombastus	Anionic hydrophilic cream DAB	276331	2
Bombastus	Anionic hydrophilic cream DAB	277297	2
Bombastus	Anionic hydrophilic cream DAB	276322	1
Bombastus	Anionic hydrophilic cream DAB	277298	2
Bombastus	Anionic hydrophilic cream DAB	277455	1
Gehe 14.05.2013	Anionic hydrophilic cream DAB	277297	1
Bombastus	Anionic hydrophilic cream DAB	277457	6
Bombastus	Anionic hydrophilic cream DAB	277458	2
Bombastus	Anionic hydrophilic cream DAB	277459	2
Bombastus	Anionic hydrophilic cream DAB	277461	3
Bombastus	Anionic hydrophilic cream DAB	277465	2
Bombastus	Anionic hydrophilic cream DAB	278846	1
Bombastus	Anionic hydrophilic cream DAB	278852	2
Caelo	Anionic hydrophilic cream DAB	278851	1
Bombastus	Anionic hydrophilic cream DAB	279055	6
Bombastus	Anionic hydrophilic cream DAB	279054	2
Bombastus	Anionic hydrophilic cream DAB	279056	2
Bombastus	Anionic hydrophilic cream DAB	279057	1
Bombastus	Anionic hydrophilic cream DAB	280289	4
Bombastus	Anionic hydrophilic cream DAB	280294	1
Caelo	Anionic hydrophilic cream DAB	28031319	1
Bombastus	Anionic hydrophilic cream DAB	280417	2
Bombastus	Anionic hydrophilic cream DAB	281999	1
Bombastus	Anionic hydrophilic cream DAB	282001	1
Gehe	Anionic hydrophilic cream DAB	282001	1
Gehe	Anionic hydrophilic cream DAB	280418	2
Bombastus	Anionic hydrophilic cream DAB	282002	1
Caelo	Anionic hydrophilic cream DAB	282005	1
Bombastus	Anionic hydrophilic cream DAB	282005	3
Bombastus	Anionic hydrophilic cream DAB	282006	2
Gehe	Anionic hydrophilic cream DAB	282111	2
Bombastus	Anionic hydrophilic cream DAB	283410	2
Bombastus	Anionic hydrophilic cream DAB	282115	1
Bombastus	Anionic hydrophilic cream DAB	282113	1
Bombastus	Anionic hydrophilic cream DAB	283481	5
Phoenix	Anionic hydrophilic cream DAB	286498	1
Caelo	Anionic hydrophilic cream SR...	2906212540	1
Bombastus	Anionic hydrophilic cream DAB	286499	2
Caelo	Anionic hydrophilic cream DAB	30081303	1
Caelo	Anionic hydrophilic cream SR...	3101212540	1
Bombastus	Anionic hydrophilic cream DAB	60080602	1
Caelo	Anionic hydrophilic cream DAB	4313I-02540	1
Phönix Gotha	Anionic hydrophilic cream SR...	4580690	1
Bombastus	Anionic hydrophilic cream DAB	6861306	1
Caelo	Anionic hydrophilic cream DAB	654879	1

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Supplier	Substance	Batch	Spectra
Caelo	Base cream, hydrophobic DAC	123588	1
Caelo	Base cream, hydrophobic DAC	13176002	2
Fagron	Base cream, hydrophobic DAC	13E13-T06-006	2
Fagron	Base cream, hydrophobic DAC	13T13-T06-006166	1
Caelo	Base cream, hydrophobic DAC	14000601	6
Hedinger/Noweda	Base cream, hydrophobic DAC	1401601	1
Caelo	Base cream, hydrophobic DAC	14028002	2
Caelo	Base cream, hydrophobic DAC	1406140	1
Caelo	Base cream, hydrophobic DAC	14061402	3
PHOENIX 11.09.2014	Base cream, hydrophobic DAC	14061501	1
Phoenix	Base cream, hydrophobic DAC	14061601	2
Caelo	Base cream, hydrophobic DAC	14061601	2
Caelo	Base cream, hydrophobic DAC	140885	1
Pharmachem.Pöfneck/Phoe...	Base cream, hydrophobic DAC	140886	1
Pharmachem GmbH	Base cream, hydrophobic DAC	140885	1
Pharmachem/Gehe	Base cream, hydrophobic DAC	140886	1
Pharmachem GmbH	Base cream, hydrophobic DAC	140886	1
Pharmachem.Pöfneck/Phoe...	Base cream, hydrophobic DAC	141318	1
Pharmachem/ /Sanacorp	Base cream, hydrophobic DAC	140885	1
Pharmachem	Base cream, hydrophobic DAC	140886	2
Pharmachem/Gehe	Base cream, hydrophobic DAC	141317	1
Nachprüfung 3083	Base cream, hydrophobic DAC	141318	1
Pharmachen	Base cream, hydrophobic DAC	141318	1
PharmaChem	Base cream, hydrophobic DAC	141318	1
Fischar	Base cream, hydrophobic DAC	14145301	3
Phönix	Base cream, hydrophobic DAC	14145301	1
GEHE 08.12.2014	Base cream, hydrophobic DAC	14145301	1
Caesar&Loretz GmbH/Anzag	Base cream, hydrophobic DAC	14145301	1
Caelo	Base cream, hydrophobic DAC	14145401	17
Pharmachem/ Noweda	Base cream, hydrophobic DAC	141489	1
Pharmachem/Gehe	Base cream, hydrophobic DAC	141489	1
PHARMACHEM GMBH/ALLIANC...	Base cream, hydrophobic DAC	142154	1
Caelo	Base cream, hydrophobic DAC	14207002	2
Pharmachen	Base cream, hydrophobic DAC	142154	3
Pröfneck	Base cream, hydrophobic DAC	142154	2
Pharmachem/Noweda	Base cream, hydrophobic DAC	142154	1
Sanacorp/ Pharmachem	Base cream, hydrophobic DAC	142155	1
Caelo	Base cream, hydrophobic DAC	14277401	1
Caelo	Base cream, hydrophobic DAC	143093	1
Pharmachem/Noweda	Base cream, hydrophobic DAC	143093	1
Pharmachem	Base cream, hydrophobic DAC	143094	5
Gehe 10.03.15	Base cream, hydrophobic DAC	143094	2
Pharmachem/ Noweda	Base cream, hydrophobic DAC	143094	1
pharmachem Pöfneck	Base cream, hydrophobic DAC	143119	1
Pharmachem.Pöfneck/Phoe...	Base cream, hydrophobic DAC	143119	1
Caelo	Base cream, hydrophobic DAC	14379902	1
Caelo	Base cream, hydrophobic DAC	1435501	1
Faoron/anzag	Base cream, hydrophobic DAC	14A06-t08-009037	1
Faoron/Anzag	Base cream, hydrophobic DAC	14A06-T08-009037	4
Fagron	Base cream, hydrophobic DAC	14E06-T13-012209	1
Fagron	Base cream, hydrophobic DAC	14H04-T05-014482	4
Caelo	Base cream, hydrophobic DAC	14L18-T21-018124	1
Fagron	Base cream, hydrophobic DAC	14L18-T21-018124	1
Phoenix	Base cream, hydrophobic DAC	15001001	1
Gehe,27.0415	Base cream, hydrophobic DAC	15001003	2
AHD/Pharmachem	Base cream, hydrophobic DAC	150404	1
Pharmachem/Gehe	Base cream, hydrophobic DAC	150404	1
Caelo	Base cream, hydrophobic DAC	15/13-T01-026887	1
Pharmachem GmbH/Noweda	Base cream, hydrophobic DAC	150405	1
Caelo	Base cream, hydrophobic DAC	1504602	1

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Supplier	Substance	Batch	Spectra
Phönix 01.06.15	Base cream, hydrophobic DAC	15048701	2
Caelo	Base cream, hydrophobic DAC	15048702	1
Caesar & Loretz GmbH	Base cream, hydrophobic DAC	15111402	1
Caelo	Base cream, hydrophobic DAC	15111403	2
Bombastus	Base cream, hydrophobic DAC	15111403	2
Pharmachem/Alliance He...	Base cream, hydrophobic DAC	151258	1
Pharmachem	Base cream, hydrophobic DAC	151258	2
Pharmachem./ Phoenix	Base cream, hydrophobic DAC	151259	1
Pharmachem GmbH	Base cream, hydrophobic DAC	151259	1
Caelo	Base cream, hydrophobic DAC	15132503	2
Pharmachem/ Alliance He...	Base cream, hydrophobic DAC	152209	1
Pharmachem /Phönix	Base cream, hydrophobic DAC	152209	1
AHD/Pharmachem	Base cream, hydrophobic DAC	152210	1
Pharmachem	Base cream, hydrophobic DAC	152209	1
Caesar&Loretz GmbH /Anzag	Base cream, hydrophobic DAC	15221301	1
Caesar&Loretz GmbH	Base cream, hydrophobic DAC	15221301	1
Caelo	Base cream, hydrophobic DAC	15221401	5
Caelo	Base cream, hydrophobic DAC	1522301	1
AHD/Pharmachem	Base cream, hydrophobic DAC	153625	2
Pharmachem	Base cream, hydrophobic DAC	153626	2
Pharmachem /Phönix	Base cream, hydrophobic DAC	153627	1
Pharmachem GmbH & CoKG	Base cream, hydrophobic DAC	153627	1
Fagron	Base cream, hydrophobic DAC	15421401	1
Caesar & Loretz GmbH	Base cream, hydrophobic DAC	15421201	1
Pharmachem GmbH & CoKG	Base cream, hydrophobic DAC	1600825	1
pharmachem	Base cream, hydrophobic DAC	160130	1
Caelo	Base cream, hydrophobic DAC	160130	2
Pharmachem GmbH & CoKG	Base cream, hydrophobic DAC	160136	1
Caelo	Base cream, hydrophobic DAC	16074801	2
Caesar & Loretz GmbH	Base cream, hydrophobic DAC	16074901	1
Caesar & Loretz/Noweda	Base cream, hydrophobic DAC	16074802	1
Caesar & Loretz/AHD	Base cream, hydrophobic DAC	16074901	1
Caesar & Loretz	Base cream, hydrophobic DAC	16075201	1
Pharmachem/Phönix	Base cream, hydrophobic DAC	160814	1
Pharmachem GmbH & CoKG	Base cream, hydrophobic DAC	160814	1
Pharmachem GmbH Pöckneck	Base cream, hydrophobic DAC	160825	1
Pharmachem Pöckneck/Phönix	Base cream, hydrophobic DAC	160825	1
Pharmachem	Base cream, hydrophobic DAC	160826	1
Noweda	Base cream, hydrophobic DAC	16165403	1
Caelo	Base cream, hydrophobic DAC	16165701	2
PHÖNIX	Base cream, hydrophobic DAC	16165701	1
Phoenix	Base cream, hydrophobic DAC	16174201	1
Caelo	Base cream, hydrophobic DAC	16174201	3
Caelo	Base cream, hydrophobic DAC	162168	1
Pharmachem/Gehe	Base cream, hydrophobic DAC	231213	1
Caelo	Base cream, hydrophobic DAC	18031505	1
Caelo	Base cream, hydrophobic DAC	26011603	1
Bombastus	Base cream, hydrophobic DAC	284171	1
Bombastus	Base cream, hydrophobic DAC	285435	1
Bombastus	Base cream, hydrophobic DAC	285434	1
Bombastus	Base cream, hydrophobic DAC	285437	2
Bombastus	Base cream, hydrophobic DAC	288497	4
Caelo	Base cream, hydrophobic DAC	289720	1
Bombastus	Base cream, hydrophobic DAC	289720	1
Bombastus	Base cream, hydrophobic DAC	291593	2
Bombastus	Base cream, hydrophobic DAC	293162	2
Caelo	Base cream, hydrophobic DAC	293162	1
Bombastus	Base cream, hydrophobic DAC	294685	3
Bombastus	Base cream, hydrophobic DAC	294686	2
Bombastus	Base cream, hydrophobic DAC	297043	1

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Supplier	Substance	Batch	Spectra
Bombastus	Base cream, hydrophobic DAC	297046	2
Bombastus	Base cream, hydrophobic DAC	297047	2
Bombastus	Base cream, hydrophobic DAC	298351	1
Bombastus	Base cream, hydrophobic DAC	298354	1
Bombastus	Base cream, hydrophobic DAC	303377	1
Sanacorp	Base cream, hydrophobic DAC	4/AKD3	1
Bombastus	Base cream, hydrophobic DAC	269276	1
Caelo	Base cream, hydrophobic DAC		10
Bombastus	Base cream, hydrophobic DAC	271091	1
Caelo	Base cream, hydrophobic DAC	5013q-03497	1
Bombastus	Base cream, hydrophobic DAC		1
Caelo	Base cream, hydrophobic DAC	46074802	1
Bombastus	Base cream, hydrophobic DAC	271093	1
Ahd/PharmachemPößneck	Base cream, hydrophobic DAC	21013	1
Pharmachem/30	Base cream, hydrophobic DAC	21013	1
Bombastus	Base cream, hydrophobic DAC	271095	1
Pharmachen	Base cream, hydrophobic DAC	21013	1
Caelo	Base cream, hydrophobic DAC	2111201	1
Phoenix/Pharmachem	Base cream, hydrophobic DAC	110413	1
PharmaChem	Base cream, hydrophobic DAC	110413	1
Fagron	Base cream, hydrophobic DAC	513A-03497	1
pharmachem	Base cream, hydrophobic DAC	110413	1
Caelo	Base cream, hydrophobic DAC	12064047	1
Pharmachem/Gehe	Base cream, hydrophobic DAC	120712	2
PharmaChem / Noweda	Base cream, hydrophobic DAC	120712	1
Erika apotheke	Base cream, hydrophobic DAC	12151601	1
Noweda/ Ichtyol	Base cream, hydrophobic DAC	12151601	2
Caelo	Base cream, hydrophobic DAC	12217603	6
Noweda	Base cream, hydrophobic DAC	12229302	4
Bombastus	Base cream, hydrophobic DAC	12229302	1
Caelo	Base cream, hydrophobic DAC	12229304	2
AHD, 02.04.2013	Base cream, hydrophobic DAC	12308102	1
Sanacorp	Base cream, hydrophobic DAC	12308102	1
Caelo	Base cream, hydrophobic DAC	12308103	2
Phönix	Base cream, hydrophobic DAC	1230822	1
Caelo	Base cream, hydrophobic DAC	123082011	1
Fagron	Base cream, hydrophobic DAC	12D10-T02	1
Fagron	Base cream, hydrophobic DAC	12G09-T03	1
Kehr	Base cream, hydrophobic DAC	12G09-T03	1
Kehr	Base cream, hydrophobic DAC	12G09-To3	1
Caesar & Loretz GmbH, 4...	Base cream, hydrophobic DAC	13019303	1
Taoasis	Base cream, hydrophobic DAC	130719-3198	1
Caelo	Base cream, hydrophobic DAC	13085504	3
Phönix	Base cream, hydrophobic DAC	13085701	2
Gehe	Base cream, hydrophobic DAC	13085701	1
Caelo	Base cream, hydrophobic DAC	13086701	1
Caelo	Base cream, hydrophobic DAC	13085702	1
Pharmachem	Base cream, hydrophobic DAC	131211	1
Caelo	Base cream, hydrophobic DAC	13127502	2
Phoenix	Base cream, hydrophobic DAC	13175902	1
Caelo	Base cream, hydrophobic DAC	13176003	7
cealo	Base cream, hydrophobic DAC	13274902	1
Caelo	Base cream, hydrophobic DAC	13275302	6
Caesar&lorenz,Phoenix	Base cream, hydrophobic DAC	13386401	1
Fagron	Base cream, hydrophobic DAC	13B04-T17-001040	2
Fagron	Base cream, hydrophobic DAC	13E13T01003619	1
Fagron	Base cream, hydrophobic DAC	13E13-T01-003620	3
Fagron	Base cream, hydrophobic DAC	13H13T06	1
Caelo	Base cream, hydrophobic DAC	1400601	1
pharmachem	Base cream, hydrophobic DAC	140886	1

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Supplier	Substance	Batch	Spectra
Caesar&loretz,Phoenix	Base cream, hydrophobic DAC	15001002	1
Phönix	Base cream, hydrophobic DAC	15111401	3
Pharmachem.Pößneck/Phoe...	Base cream, hydrophobic DAC	230713	1
Pharmachem / Anzag	Base cream, hydrophobic DAC	230713	2
Pharmachem	Base cream, hydrophobic DAC	230713	1
Pharmachem/Noweda	Base cream, hydrophobic DAC	231213	1
Pharmachem/Noweda	Base cream, hydrophobic DAC	230713	1
PharmaChin/ Anzag	Base cream, hydrophobic DAC	230713	1
pharmachem	Base cream, hydrophobic DAC	231213	1
Pharmachen	Base cream, hydrophobic DAC	231213	1
pharmachen	Base cream, hydrophobic DAC	240113	1
Pharmachen	Base cream, hydrophobic DAC	240113	1
Gehe	Base cream, hydrophobic DAC	261112	1
Pharmachem / Anzag	Base cream, hydrophobic DAC	240113	1
Pharmachem Pößneck 004	Base cream, hydrophobic DAC	261112	1
Pharmachen Pößneck	Base cream, hydrophobic DAC	261112	1
Hersteller: Pharmachem/...	Base cream, hydrophobic DAC	261112	2
Pharmachem GmbH	Base cream, hydrophobic DAC	261112	1
Pharmachem / Anzag	Base cream, hydrophobic DAC	261112	1
Bombastus	Base cream, hydrophobic DAC	276087	1
Phönix Gotha	Base cream, hydrophobic DAC	277696	1
Bombastus	Base cream, hydrophobic DAC	277696	1
Bombastus	Base cream, hydrophobic DAC	279145	2
Bombastus	Base cream, hydrophobic DAC	279148	2
Bombastus	Base cream, hydrophobic DAC	280809	1
Bombastus	Base cream, hydrophobic DAC	282161	1
Bombastus	Base cream, hydrophobic DAC	284170	1
Bombastus	Base cream, hydrophobic DAC	282162	1
Caelo	Base cream, hydrophobic DAC	410211-1-P	1
Noweda	Base cream, hydrophobic DAC	11289203	1
Pößneck Pharmachem	Base cream, hydrophobic DAC	131011	1
gehe	Hydrophilic cream, non-ionic...	1B070114	1
GEHE/Apomix/25.03.2014	Hydrophilic cream, non-ionic...	1A140114	1
Apomix	Hydrophilic cream, non-ionic...	1A200116	1
apomix/Noweda	Hydrophilic cream, non-ionic...	1A210115	1
Apomix	Hydrophilic cream, non-ionic...	1A210115	1
Gehe/Apomix	Hydrophilic cream, non-ionic...	2A140114	2
Apomix/Noweda	Hydrophilic cream, non-ionic...	2A090215	1
Apomix / AHD	Hydrophilic cream, non-ionic...	2A140114	2
apomix/Phönix	Hydrophilic cream, non-ionic...	3A090215	1
Apomix/Gehe	Hydrophilic cream, non-ionic...	3B020215	1
Apomix / Noweda	Hydrophilic cream, non-ionic...	3B020215	1
APOMIX/Noweda	Hydrophilic cream, non-ionic...	4a230216	1
Apomix/Noweda	Hydrophilic cream, non-ionic...	4A240215	1
Apomix / Phönix	Hydrophilic cream, non-ionic...	4A250214	2
Raben-Apotheke Mildenau	Hydrophilic cream, non-ionic...	4B100214	1
Apomix	Hydrophilic cream, non-ionic...	4B170216	1
Gehe/Apomix/11.11.14	Hydrophilic cream, non-ionic...	4A250214	1
Apomix	Hydrophilic cream, non-ionic...	6B020315	1
Apomix	Hydrophilic cream, non-ionic...	6B100314	1
Apomix / Sanacorp	Hydrophilic cream, non-ionic...	6B020315	1
Pharmachem	Hydrophilic cream, non-ionic...	6B150316	1
Apomix	Hydrophilic cream, non-ionic...	7A020414	1
Apomix/Noweda	Hydrophilic cream, non-ionic...	7A020414	1
Apomix / Phönix	Hydrophilic cream, non-ionic...	7A020414	1
Apomix	Hydrophilic cream, non-ionic...	8B070414	1
Gehe/apomix/09.10.14	Hydrophilic cream, non-ionic...	7A020414	1
apomix/Phönix	Hydrophilic cream, non-ionic...	8B070414	1
apomix/Noweda	Hydrophilic cream, non-ionic...	7A310316	1
Pharmachem/Phoenix	Hydrophilic cream, non-ionic...	90714	1

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Supplier	Substance	Batch	Spectra
Noweda	Hydrophilic cream, non-ionic...	90714	1
Apomix / Noweda	Hydrophilic cream, non-ionic...	9B200415	1
Apomix	Hydrophilic cream, non-ionic...	9B020516	1
Phönix Gotha	Hydrophilic cream, non-ionic...	10B200415	1
Apomix/Noweda	Hydrophilic cream, non-ionic...	10B200415	1
apomix	Hydrophilic cream, non-ionic...	10B190516	1
Apomix	Hydrophilic cream, non-ionic...	11B110515	1
Apomix	Hydrophilic cream, non-ionic...	10B190516	1
Fagron	Hydrophilic cream, non-ionic...	12A020315	1
PKH GmbH	Hydrophilic cream, non-ionic...	12B1306161	1
Bombastus	Hydrophilic cream, non-ionic...	12B130626	1
Fagron	Hydrophilic cream, non-ionic...	12A180416	1
Raben-Apotheke Mildenau	Hydrophilic cream, non-ionic...	12B210514	1
Apomix / Sanacorp	Hydrophilic cream, non-ionic...	12B210514	1
Leyh Pharma/ Phönix	Hydrophilic cream, non-ionic...	133911	2
Leyh Pharma	Hydrophilic cream, non-ionic...	134841	1
Fagron	Hydrophilic cream, non-ionic...	13A180416	1
Apomix	Hydrophilic cream, non-ionic...	13B080615	2
apomix	Hydrophilic cream, non-ionic...	13B280616	2
Fagron	Hydrophilic cream, non-ionic...	13K15-M09	1
Fagron	Hydrophilic cream, non-ionic...	13K20-M10	1
Fagron	Hydrophilic cream, non-ionic...	13K20-M09	1
Leyh Pharma/Gehe	Hydrophilic cream, non-ionic...	140551	1
Fagron	Hydrophilic cream, non-ionic...	13K20-M11	1
Caelo	Hydrophilic cream, non-ionic...	14063001	1
Caelo	Hydrophilic cream, non-ionic...	14063003	1
Caelo	Hydrophilic cream, non-ionic...	14137002	3
Caelo	Hydrophilic cream, non-ionic...	14221101	1
Phönix/Leyh Pharma	Hydrophilic cream, non-ionic...	142311	1
Leyh Pharma / Phönix	Hydrophilic cream, non-ionic...	142311	1
Leyh Pharma/Phönix	Hydrophilic cream, non-ionic...	143011	1
Leyh/Gehe	Hydrophilic cream, non-ionic...	143011	2
Caelo	Hydrophilic cream, non-ionic...	14336001	1
Fagron	Hydrophilic cream, non-ionic...	14D28-M02	1
Fagron	Hydrophilic cream, non-ionic...	14D28-M05	2
Fagron	Hydrophilic cream, non-ionic...	14D28-M03	1
Fagron	Hydrophilic cream, non-ionic...	14D28-M05	1
Fagron	Hydrophilic cream, non-ionic...	14E07-M10	1
Fagron	Hydrophilic cream, non-ionic...	14D28-Mo9	1
Fagron	Hydrophilic cream, non-ionic...	14E14-M06	1
Phönix Gotha	Hydrophilic cream, non-ionic...	150341	1
Gehe/Leyh	Hydrophilic cream, non-ionic...	150341	1
Caelo	Hydrophilic cream, non-ionic...	15325802	1
Caelo	Hydrophilic cream, non-ionic...	15365601	2
Fagron	Hydrophilic cream, non-ionic...	15A-200416	1
Apomix/ Phönix	Hydrophilic cream, non-ionic...	15B070714	1
Caelo	Hydrophilic cream, non-ionic...	16017501	4
PKH Halle	Hydrophilic cream, non-ionic...	15B080816	1
Apomix/ Phönix	Hydrophilic cream, non-ionic...	15B090713	1
Caelo	Hydrophilic cream, non-ionic...	16169501	1
Caelo	Hydrophilic cream, non-ionic...	16222001	1
Apomix	Hydrophilic cream, non-ionic...	17B120814	2
Gehe/Apomix	Hydrophilic cream, non-ionic...	18A190315	1
Apomix / Sanacorp	Hydrophilic cream, non-ionic...	18B240815	1
Raben-Apotheke Mildenau	Hydrophilic cream, non-ionic...	18B020914	2
apomix noweder 23.10.2015	Hydrophilic cream, non-ionic...	18B240815	1
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	19A300315	1
Caelo	Hydrophilic cream, non-ionic...	201015	2
Apomix/NOWEDA	Hydrophilic cream, non-ionic...	19A300315	1
apomix	Hydrophilic cream, non-ionic...	19A300315	1

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Supplier	Substance	Batch	Spectra
apomix/Phönix	Hydrophilic cream, non-ionic...	19A300315	1
PKH Halle/Noweda	Hydrophilic cream, non-ionic...	20A280415	1
Apomix/Gehe	Hydrophilic cream, non-ionic...	20B210915	1
Apomix/ Phönix	Hydrophilic cream, non-ionic...	20B230913	1
Apomix	Hydrophilic cream, non-ionic...	20B290914	2
Phönix Gotha	Hydrophilic cream, non-ionic...	21B141014	1
PKH GmbH	Hydrophilic cream, non-ionic...	21B141116	2
Caelo	Hydrophilic cream, non-ionic...	21B141116	1
Pharmachem/Phoenix	Hydrophilic cream, non-ionic...	220713	12
Pharmachem / Phönix	Hydrophilic cream, non-ionic...	220713	1
apomix/Phönix	Hydrophilic cream, non-ionic...	23A100615	1
apomix/Phönix	Hydrophilic cream, non-ionic...	22B061114	1
Apomix	Hydrophilic cream, non-ionic...	23A280416	2
apomix	Hydrophilic cream, non-ionic...	24B241115	1
Apomix/Sana	Hydrophilic cream, non-ionic...	25B081215	1
Bombastus	Hydrophilic cream, non-ionic...	276593	1
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	26A080715	1
PKH/Noweda	Hydrophilic cream, non-ionic...	27A220715	1
gehe	Hydrophilic cream, non-ionic...	280990	1
Bombastus	Hydrophilic cream, non-ionic...	282215	2
Caesar & Loretz GmbH Hi...	Hydrophilic cream, non-ionic...	282216	1
Bombastus	Hydrophilic cream, non-ionic...	282216	5
Bombastus	Hydrophilic cream, non-ionic...	283634	1
Bombastus	Hydrophilic cream, non-ionic...	283636	4
Caelo	Hydrophilic cream, non-ionic...	283634	1
Bombastus	Hydrophilic cream, non-ionic...	284891	3
Bombastus	Hydrophilic cream, non-ionic...	283639	1
Bombastus	Hydrophilic cream, non-ionic...	283695	1
Bombastus	Hydrophilic cream, non-ionic...	283635	2
gehe	Hydrophilic cream, non-ionic...	283693	1
Bombastus	Hydrophilic cream, non-ionic...	284893	2
Bombastus	Hydrophilic cream, non-ionic...	284895	4
Bombastus	Hydrophilic cream, non-ionic...	284896	1
Bombastus	Hydrophilic cream, non-ionic...	284898	2
Herbasinica	Hydrophilic cream, non-ionic...	284899	1
Bombastus	Hydrophilic cream, non-ionic...	286323	1
Hedinger	Hydrophilic cream, non-ionic...	286326	1
Caelo	Hydrophilic cream, non-ionic...	286327	1
Bombastus	Hydrophilic cream, non-ionic...	286329	2
Bombastus	Hydrophilic cream, non-ionic...	286330	3
Gehe 02.09.14	Hydrophilic cream, non-ionic...	287709	1
Bombastus	Hydrophilic cream, non-ionic...	287710	2
Bombastus	Hydrophilic cream, non-ionic...	287711	6
Bombastus	Hydrophilic cream, non-ionic...	287713	3
Bombastus	Hydrophilic cream, non-ionic...	287715	2
Bombastus	Hydrophilic cream, non-ionic...	288793	1
Bombastus	Hydrophilic cream, non-ionic...	288795	2
Bombastus	Hydrophilic cream, non-ionic...	288882	1
Bombastus	Hydrophilic cream, non-ionic...	288798	1
Bombastus	Hydrophilic cream, non-ionic...	288796	1
Bombastus	Hydrophilic cream, non-ionic...	289326	1
Bombastus	Hydrophilic cream, non-ionic...	289937	1
Gehe	Hydrophilic cream, non-ionic...	289937	1
Bombastus	Hydrophilic cream, non-ionic...	289940	1
Gehe	Hydrophilic cream, non-ionic...	289941	1
Bombastus	Hydrophilic cream, non-ionic...	289941	1
Bombastus	Hydrophilic cream, non-ionic...	289943	2
Bombastus	Hydrophilic cream, non-ionic...	289942	2
Caelo	Hydrophilic cream, non-ionic...	289944	1
Bombastus	Hydrophilic cream, non-ionic...	291382	1

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Supplier	Substance	Batch	Spectra
Bombastus	Hydrophilic cream, non-ionic...	291386	1
Caelo	Hydrophilic cream, non-ionic...	291388	1
Euro OTC	Hydrophilic cream, non-ionic...	291388	1
Bombastus	Hydrophilic cream, non-ionic...	291388	4
Bombastus	Hydrophilic cream, non-ionic...	292737	1
Bombastus	Hydrophilic cream, non-ionic...	292738	1
Bombastus	Hydrophilic cream, non-ionic...	292740	1
Bombastus	Hydrophilic cream, non-ionic...	292811	1
Bombastus	Hydrophilic cream, non-ionic...	292808	1
Bombastus	Hydrophilic cream, non-ionic...	292810	1
Bombastus	Hydrophilic cream, non-ionic...	292812	1
Bombastus	Hydrophilic cream, non-ionic...	294311	2
Bombastus	Hydrophilic cream, non-ionic...	294310	1
Caelo	Hydrophilic cream, non-ionic...	294310	1
Bombastus	Hydrophilic cream, non-ionic...	294313	1
Bombastus	Hydrophilic cream, non-ionic...	294390	1
Bombastus	Hydrophilic cream, non-ionic...	294340	1
Bombastus	Hydrophilic cream, non-ionic...	294408	3
Bombastus	Hydrophilic cream, non-ionic...	295591	1
Bombastus / Noweda	Hydrophilic cream, non-ionic...	295647	1
Bombastus	Hydrophilic cream, non-ionic...	295648	1
Bombastus	Hydrophilic cream, non-ionic...	295649	2
Bombastus	Hydrophilic cream, non-ionic...	295651	1
Bombastus	Hydrophilic cream, non-ionic...	295655	5
Bombastus	Hydrophilic cream, non-ionic...	295654	1
Bombastus	Hydrophilic cream, non-ionic...	295657	4
Bombastus	Hydrophilic cream, non-ionic...	297308	3
Bombastus	Hydrophilic cream, non-ionic...	297303	1
Bombastus	Hydrophilic cream, non-ionic...	297310	1
Noweda	Hydrophilic cream, non-ionic...	297309	1
Bombastus	Hydrophilic cream, non-ionic...	297372	1
Bombastus	Hydrophilic cream, non-ionic...	297371	1
Bombastus	Hydrophilic cream, non-ionic...	297374	1
Bombastus	Hydrophilic cream, non-ionic...	298979	1
Bombastus	Hydrophilic cream, non-ionic...	298982	1
Bombastus	Hydrophilic cream, non-ionic...	298981	1
Bombastus	Hydrophilic cream, non-ionic...	300035	2
Bombastus	Hydrophilic cream, non-ionic...	298983	2
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	29A110815	1
Bombastus	Hydrophilic cream, non-ionic...	2x295649	1
Phoenix	Hydrophilic cream, non-ionic...	300035	1
Bombastus	Hydrophilic cream, non-ionic...	300756	1
Bombastus	Hydrophilic cream, non-ionic...	300764	2
Bombastus	Hydrophilic cream, non-ionic...	300765	1
Bombastus	Hydrophilic cream, non-ionic...	30162	1
Bombastus	Hydrophilic cream, non-ionic...	301627	2
Bombastus	Hydrophilic cream, non-ionic...	302686	1
Bombastus	Hydrophilic cream, non-ionic...	302687	1
Bombastus	Hydrophilic cream, non-ionic...	302688	2
Bombastus	Hydrophilic cream, non-ionic...	304775	1
Bombastus	Hydrophilic cream, non-ionic...	304778	2
Bombastus	Hydrophilic cream, non-ionic...	304776	1
Bombastus	Hydrophilic cream, non-ionic...	304777	1
GEHE/Apomix/04.02.14	Hydrophilic cream, non-ionic...	30A030613	2
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	32A220915	1
Apomix/AHD/24.06.14	Hydrophilic cream, non-ionic...	32A250414	1
apomix	Hydrophilic cream, non-ionic...	32A220915	1
apomix/Holdermann	Hydrophilic cream, non-ionic...	32A250414	2
Fagron	Hydrophilic cream, non-ionic...	33A180912	2
AMH Niemann GmbH & Co. KG	Hydrophilic cream, non-ionic...	34A210916	1

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Supplier	Substance	Batch	Spectra
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	36A140514	1
AHD/apomix/23.07.14	Hydrophilic cream, non-ionic...	36A140514	1
Apomix	Hydrophilic cream, non-ionic...	36A140514a	1
Raben-Apotheke Mildenau	Hydrophilic cream, non-ionic...	37A270514	1
Apomix	Hydrophilic cream, non-ionic...	40A160614	1
Apomix/Noweda	Hydrophilic cream, non-ionic...	39A160614	1
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	40A160614	1
Anzag/apomix/26.03.14	Hydrophilic cream, non-ionic...	40A281013	1
Fagron	Hydrophilic cream, non-ionic...	4315A-03195	1
apomix/Holdermann	Hydrophilic cream, non-ionic...	43A140714	1
Apomix	Hydrophilic cream, non-ionic...	48A081014	1
Fagron	Hydrophilic cream, non-ionic...	48A071113	1
Gehe/apomix/11.12.14	Hydrophilic cream, non-ionic...	48A081014	1
apomix/Phönix	Hydrophilic cream, non-ionic...	47A281015	1
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	47A281015	1
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	48A081014	1
Apomix	Hydrophilic cream, non-ionic...	49A241115	1
Fagron	Hydrophilic cream, non-ionic...	51A121113	2
Apomix/Noweda	Hydrophilic cream, non-ionic...	50A161215	1
Apomix	Hydrophilic cream, non-ionic...	51A261114	1
Fagron	Hydrophilic cream, non-ionic...	5214I-03195	1
apomix/Gehe	Hydrophilic cream, non-ionic...	51A261114	1
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	52A081214	1
Apomix / AHD	Hydrophilic cream, non-ionic...	53A021213	1
Apomix/Sanacorp	Hydrophilic cream, non-ionic...	53A191113	1
Phönix	Hydrophilic cream, non-ionic...		1
Bombastus	Hydrophilic cream, non-ionic...	253825	1
Bombastus	Hydrophilic cream, non-ionic...	264427	1
Bombastus	Hydrophilic cream, non-ionic...	267068	1
Apomix/Noweda	Hydrophilic cream, non-ionic...	54A021213	1
Bombastus	Hydrophilic cream, non-ionic...	267185	2
Caelo	Hydrophilic cream, non-ionic...	267186	1
Bombastus	Hydrophilic cream, non-ionic...	268349	1
Bombastus	Hydrophilic cream, non-ionic...	268353	1
Bombastus	Hydrophilic cream, non-ionic...	269711	1
Bombastus	Hydrophilic cream, non-ionic...	269712	1
Bombastus	Hydrophilic cream, non-ionic...	271520	1
Bombastus	Hydrophilic cream, non-ionic...	271518	1
Bombastus	Hydrophilic cream, non-ionic...	269715	1
Gehe	Hydrophilic cream, non-ionic...	271520	2
Bombastus	Hydrophilic cream, non-ionic...	269716	1
Bombastus	Hydrophilic cream, non-ionic...	271521	2
Gehe	Hydrophilic cream, non-ionic...	271521	1
Bombastus	Hydrophilic cream, non-ionic...	272472	1
Bombastus	Hydrophilic cream, non-ionic...	273132	1
Bombastus	Hydrophilic cream, non-ionic...	273137	1
Bombastus	Hydrophilic cream, non-ionic...	274212	1
Bombastus	Hydrophilic cream, non-ionic...	274213	1
Gehe	Hydrophilic cream, non-ionic...	274215	1
Bombastus	Hydrophilic cream, non-ionic...	274216	2
Bombastus	Hydrophilic cream, non-ionic...	274217	2
Bombastus	Hydrophilic cream, non-ionic...	274222	1
Apomix	Hydrophilic cream, non-ionic...	1A030113	1
Apomix	Hydrophilic cream, non-ionic...	1A030112	1
Apomix/Alliance Healthc...	Hydrophilic cream, non-ionic...	8/14	1
Apomix / AHD	Hydrophilic cream, non-ionic...	1A030113	2
APOMIX /11	Hydrophilic cream, non-ionic...	1B070114	1
apomix	Hydrophilic cream, non-ionic...	2A140113	1
Apomix	Hydrophilic cream, non-ionic...	2A140113	1
apomix/GEHE/22.05.2013	Hydrophilic cream, non-ionic...	2A140113	1

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Supplier	Substance	Batch	Spectra
apomix	Hydrophilic cream, non-ionic...	2B140113	1
Phönix/ Apomix	Hydrophilic cream, non-ionic...	2B160412	1
Phönix/ Apomix	Hydrophilic cream, non-ionic...	2B140113	1
apomix	Hydrophilic cream, non-ionic...	3A240413	1
Pharmachem/Phoenix	Hydrophilic cream, non-ionic...	50912	4
apo	Hydrophilic cream, non-ionic...	4807013	1
Phönix/ Apomix	Hydrophilic cream, non-ionic...	3B230112	1
Apomix	Hydrophilic cream, non-ionic...	5B250213	1
Gehe	Hydrophilic cream, non-ionic...	5B250213	1
Apomix	Hydrophilic cream, non-ionic...	6B110313	1
AMH Niemann	Hydrophilic cream, non-ionic...	7B020413	2
Fagron	Hydrophilic cream, non-ionic...	5A230113	1
apomix GmbH/Phönix	Hydrophilic cream, non-ionic...	7B020413	1
Pharmachem	Hydrophilic cream, non-ionic...	80611	1
AMH Niemann/K	Hydrophilic cream, non-ionic...	10A190312	1
Apomix	Hydrophilic cream, non-ionic...	9B300413	1
apomix	Hydrophilic cream, non-ionic...	9A060213	1
Apomix	Hydrophilic cream, non-ionic...	10B220513	1
Apomix / Phönix	Hydrophilic cream, non-ionic...	11A040313	1
Gehe	Hydrophilic cream, non-ionic...	114761	1
Anzag	Hydrophilic cream, non-ionic...	114761	1
Apomix	Hydrophilic cream, non-ionic...	11A040313	1
Apomix/Gehe GUC	Hydrophilic cream, non-ionic...	11B220513	1
Fagron	Hydrophilic cream, non-ionic...	12/26-M06	1
Gehe	Hydrophilic cream, non-ionic...	120211	1
Gehe	Hydrophilic cream, non-ionic...	122131	1
Phönix Gotha	Hydrophilic cream, non-ionic...	123711	1
Phönix Gotha	Hydrophilic cream, non-ionic...	125011	3
Gehe	Hydrophilic cream, non-ionic...	125011	1
Leyh Pharma	Hydrophilic cream, non-ionic...	125011	1
Apomix	Hydrophilic cream, non-ionic...	12A040313	3
Apomix/Alliance Healthc...	Hydrophilic cream, non-ionic...	12A040313	1
All..Healthc./Apomix	Hydrophilic cream, non-ionic...	12A040313	1
AMH Niemann GmbH& Co. K...	Hydrophilic cream, non-ionic...	12B030613	2
Anzag, 12.09.2012	Hydrophilic cream, non-ionic...	12G19-M07	1
Fagron	Hydrophilic cream, non-ionic...	12J04-M06	2
Fagron	Hydrophilic cream, non-ionic...	12I26-M05	1
Großhandel	Hydrophilic cream, non-ionic...	12I26-M06	1
Phönix Gotha	Hydrophilic cream, non-ionic...	130651	3
Phönix Gotha	Hydrophilic cream, non-ionic...	13065	1
Gehe	Hydrophilic cream, non-ionic...	131451	1
Phönix Gotha	Hydrophilic cream, non-ionic...	13227701	1
Gehe	Hydrophilic cream, non-ionic...	132331	1
Phönix	Hydrophilic cream, non-ionic...	132331	1
Phönix Gotha	Hydrophilic cream, non-ionic...	132331	2
Gehe	Hydrophilic cream, non-ionic...	133121	1
Leyh Pharma GmbH/Anzag	Hydrophilic cream, non-ionic...	133121	1
Phönix Gotha	Hydrophilic cream, non-ionic...	133911	2
Fagron	Hydrophilic cream, non-ionic...	13D05-M07	1
Fagron	Hydrophilic cream, non-ionic...	13A30-M01	1
Fagron	Hydrophilic cream, non-ionic...	13D05M08	1
Fagron	Hydrophilic cream, non-ionic...	13B06-M08	1
Fagron	Hydrophilic cream, non-ionic...	13D05-M09	1
Fagron	Hydrophilic cream, non-ionic...	13D05-M08	1
Fagron	Hydrophilic cream, non-ionic...	13D05-M12	1
Fagron	Hydrophilic cream, non-ionic...	13D18-M06	2
Großhandel	Hydrophilic cream, non-ionic...	13D18-M06	1
Fagron	Hydrophilic cream, non-ionic...	13D18-M09	2
Fagron	Hydrophilic cream, non-ionic...	13D18-M10	3
Caelo	Hydrophilic cream, non-ionic...	13k15-m09	1

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Supplier	Substance	Batch	Spectra
Anzag/AMH/16.05.2012	Hydrophilic cream, non-ionic...	14B020212	1
Phönix/ Apomix	Hydrophilic cream, non-ionic...	14B300511	1
apomix/Phönix	Hydrophilic cream, non-ionic...	15B090713	2
AMH Niemann/G	Hydrophilic cream, non-ionic...	15A140512	1
Fagron	Hydrophilic cream, non-ionic...	14D28-M04	1
Apomix	Hydrophilic cream, non-ionic...	16B290713	1
Pharmachem/Phönix	Hydrophilic cream, non-ionic...	170412	1
Apomix	Hydrophilic cream, non-ionic...	18B190612	1
Apomix	Hydrophilic cream, non-ionic...	19B260612	1
AMH Niemann/G	Hydrophilic cream, non-ionic...	20A090413	1
Apomix	Hydrophilic cream, non-ionic...	19B100913	1
Phönix Gotha	Hydrophilic cream, non-ionic...	20B230913	2
Apomix/Noweda	Hydrophilic cream, non-ionic...	21B141013	1
Phönix Gotha	Hydrophilic cream, non-ionic...	20B260612	1
Henry Lamotte	Hydrophilic cream, non-ionic...	22B281013	2
Fagron	Hydrophilic cream, non-ionic...	24A110413	1
Apomix	Hydrophilic cream, non-ionic...	23B141113	1
Fagron	Hydrophilic cream, non-ionic...	24A110712	1
Apomix/Phönix	Hydrophilic cream, non-ionic...	25B161213	1
Apomix	Hydrophilic cream, non-ionic...	24B180912	1
Caelo	Hydrophilic cream, non-ionic...	25B240912	1
Apomix Anzag	Hydrophilic cream, non-ionic...	25A120712	1
Bombastus	Hydrophilic cream, non-ionic...	271397	1
Apomix	Hydrophilic cream, non-ionic...	26B151012	1
Gehe	Hydrophilic cream, non-ionic...	271397	1
Bombastus	Hydrophilic cream, non-ionic...	273128	1
Gehe	Hydrophilic cream, non-ionic...	274101	1
Bombastus	Hydrophilic cream, non-ionic...	276597	2
Gehe	Hydrophilic cream, non-ionic...	276599	1
Bombastus	Hydrophilic cream, non-ionic...	276599	2
Bombastus	Hydrophilic cream, non-ionic...	276595	1
Bombastus	Hydrophilic cream, non-ionic...	276598	2
Bombastus	Hydrophilic cream, non-ionic...	276600	1
Bombastus	Hydrophilic cream, non-ionic...	276725	2
Gehe	Hydrophilic cream, non-ionic...	277872	1
Bombastus	Hydrophilic cream, non-ionic...	277871	1
Bombastus	Hydrophilic cream, non-ionic...	277877	2
Caelo	Hydrophilic cream, non-ionic...	277877	1
Caelo	Hydrophilic cream, non-ionic...	277878	1
Bombastus	Hydrophilic cream, non-ionic...	277880	1
Caelo	Hydrophilic cream, non-ionic...	277880	1
Bombastus	Hydrophilic cream, non-ionic...	277881	1
Bombastus	Hydrophilic cream, non-ionic...	278025	5
Bombastus	Hydrophilic cream, non-ionic...	278026	2
Bombastus	Hydrophilic cream, non-ionic...	278028	3
Bombastus	Hydrophilic cream, non-ionic...	278029	1
Bombastus	Hydrophilic cream, non-ionic...	279656	2
AMH Niemann GmbH & Co. KG	Hydrophilic cream, non-ionic...	27A150513	1
Bombastus	Hydrophilic cream, non-ionic...	279991	1
apomix	Hydrophilic cream, non-ionic...	27A150513	1
Bombastus	Hydrophilic cream, non-ionic...	280984	1
Bombastus	Hydrophilic cream, non-ionic...	280986	2
Bombastus	Hydrophilic cream, non-ionic...	280987	1
Gehe	Hydrophilic cream, non-ionic...	280989	2
Bombastus	Hydrophilic cream, non-ionic...	280993	3
Bombastus	Hydrophilic cream, non-ionic...	282213	4
Gehe	Hydrophilic cream, non-ionic...	282212	1
Bombastus	Hydrophilic cream, non-ionic...	281774	1
Bombastus	Hydrophilic cream, non-ionic...	283638	1
Bombastus	Hydrophilic cream, non-ionic...	287716	1

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Supplier	Substance	Batch	Spectra
Apomix	Hydrophilic cream, non-ionic...	28B221012	1
Bombastus	Hydrophilic cream, non-ionic...	292809	1
Apomix	Hydrophilic cream, non-ionic...	30A030613	1
Apomix	Hydrophilic cream, non-ionic...	32A090713	1
Apomix	Hydrophilic cream, non-ionic...	33A051211	1
apomix	Hydrophilic cream, non-ionic...	30A170912	1
PKH Halle/ Alliance H.	Hydrophilic cream, non-ionic...	33a240713	1
PKH Halle/ Alliance H.	Hydrophilic cream, non-ionic...	33A240713	2
Alliance Healthcare/Apo...	Hydrophilic cream, non-ionic...	33A240713	1
Apomix / Noweda	Hydrophilic cream, non-ionic...	33A240713	1
Apomix	Hydrophilic cream, non-ionic...	33B271212	1
AMH Niemann GmbH & Co. KG	Hydrophilic cream, non-ionic...	35A070813	1
Apomix / Phönix	Hydrophilic cream, non-ionic...	35A070813	1
apomix/GEHE/02.07.2013	Hydrophilic cream, non-ionic...	40A261112	1
Apomix	Hydrophilic cream, non-ionic...	38A051112	1
Apomix	Hydrophilic cream, non-ionic...	42A191212	1
Apomix	Hydrophilic cream, non-ionic...	40A281013	1
Fagron	Hydrophilic cream, non-ionic...	412062-3-P	1
Apomix	Hydrophilic cream, non-ionic...	54A021213	1
Alliance Healthcare/Apo...	Hydrophilic cream, non-ionic...	55A181213	1
Bombastus	Hydrophilic cream, non-ionic...	82216	1
Fagron	Hydrophilic cream, non-ionic...	55A181213	1
Bombastus	Hydrophilic cream, non-ionic...	96914	1
Caesar &Loretz GmbH	Hydrophilic cream, non-ionic...		3
Eigene	Hydrophilic cream, non-ionic...	R12/0313	1
Fagron	Transdermal basic cream	12H17-T02-005161	2
Fagron	Transdermal basic cream	1504065	3
Fagron	Transdermal basic cream	1507997	3
Fagron	Transdermal basic cream	15A28-T10-018922	1
Fagron	Transdermal basic cream	15D28-T06-02194	1
Fagron	Transdermal basic cream	247191-0003	1
Fagron	Transdermal basic cream	12F19-U15-273303	1
Fagron	Transdermal basic cream	12H17-T02-000281	1
Fagron	Transdermal basic cream	14B27-T01-010612	3
Fagron	Transdermal basic cream	4315I-07039	1
Fagron	Transdermal basic cream	13G17-T03-005497	1
Fagron	Transdermal basic cream	13G17-T03-010523	1
Fagron	Transdermal basic cream	14C14-T03-011060	1
Fagron	Transdermal basic cream	14H19-T07-014889	1
Euro OTC	Transdermal basic cream	14J08-T12-016301	2
Fagron	Transdermal basic cream	15A28-T08-018919	1
Fagron	Transdermal basic cream	14K21-T03-017364	1
Fagron	Transdermal basic cream	14B27-T010612	1
Fagron	Transdermal basic cream	14C14-T03	1
Fagron	Transdermal basic cream	15D28-T06-021940	1
Fagron	Transdermal basic cream	1602049	1
Fagron	Transdermal basic cream	14B27-To1-010612	1
Apomix	Hydrophilic cream, non-ionic...	1A080113	2
Caelo	Anionic hydrophilic cream DAB	1315Q-02540	1
Caelo	Anionic hydrophilic cream DAB	13168201	2
Caelo	Anionic hydrophilic cream DAB	13314101	8
Fagron	Base cream, hydrophobic DAC	13B04-t17-001037	1
Caesar & Lorenz	Base cream, hydrophobic DAC	14028002	1
Caesar & Lorenz	Base cream, hydrophobic DAC	14061501	1
Caelo	Anionic hydrophilic cream DAB	14138701	3
Caelo	Anionic hydrophilic cream DAB	14186501	11
Caelo	Anionic hydrophilic cream DAB	14186101	5
Caelo	Anionic hydrophilic cream DAB	14186801	5
Caelo	Anionic hydrophilic cream wi...	14214001	5
Caelo	Anionic hydrophilic cream wi...	14214201	27

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Supplier	Substance	Batch	Spectra
pharmachem/spangro	Base cream, hydrophobic DAC	142154	1
Caelo	Anionic hydrophilic cream wi...	14214301	1
Caelo	Anionic hydrophilic cream DAB	14233201	3
Caelo	Anionic hydrophilic cream DAB	14233301	4
Caelo	Anionic hydrophilic cream DAB	14233001	3
Caelo	Anionic hydrophilic cream DAB	14285801	5
Caelo	Anionic hydrophilic cream DAB	14294201	6
Caelo	Anionic hydrophilic cream wi...	14334201	10
Caelo	Anionic hydrophilic cream DAB	14341601	5
Caelo	Anionic hydrophilic cream DAB	14341801	1
Caelo	Anionic hydrophilic cream DAB	14374801	3
Caelo	Anionic hydrophilic cream DAB	15001201	6
Sanacorp	Hydrophilic cream, non-ionic...	15039001	1
Caelo	Anionic hydrophilic cream wi...	15048401	6
Caelo	Anionic hydrophilic cream wi...	15048501	12
Caelo	Anionic hydrophilic cream wi...	15132701	4
Caelo	Anionic hydrophilic cream wi...	15132902	9
Caelo	Anionic hydrophilic cream wi...	15133001	6
Caelo	Anionic hydrophilic cream DAB	15200001	3
Caelo	Anionic hydrophilic cream wi...	15273001	20
Caelo	Anionic hydrophilic cream DAB	15267401	6
Caelo	Anionic hydrophilic cream wi...	15273301	4
Caelo	Anionic hydrophilic cream DAB	15315601	1
Caelo	Anionic hydrophilic cream DAB	15357401	2
Caelo	Anionic hydrophilic cream DAB	15400601	1
Caelo	Anionic hydrophilic cream wi...	15405201	2
Caelo	Anionic hydrophilic cream DAB	15401601	1
Caelo	Anionic hydrophilic cream wi...	15405401	10
Caelo	Anionic hydrophilic cream DAB	15431702	2
Fagron	Anionic hydrophilic cream DAB	16046701	1
Caelo	Anionic hydrophilic cream DAB	16046301	1
Caelo	Anionic hydrophilic cream DAB	16057201	1
Caelo	Anionic hydrophilic cream DAB	16057301	1
Caelo	Anionic hydrophilic cream wi...	16067701	5
Caelo	Anionic hydrophilic cream wi...	16067301	2
Caelo	Hydrophilic cream, non-ionic...	16114201	2
Caelo	Anionic hydrophilic cream DAB	16179601	1
Caelo	Anionic hydrophilic cream SR...	16258601	1
Caelo	Anionic hydrophilic cream DAB	16259601	2
Caelo	Anionic hydrophilic cream DAB	16259701	1
Pharmachem/AHD	Base cream, hydrophobic DAC	231213	2
Bombastus	Anionic hydrophilic cream DAB	283480	3
Bombastus	Anionic hydrophilic cream DAB	283483	1
Bombastus	Anionic hydrophilic cream DAB	285593	1
Bombastus	Anionic hydrophilic cream DAB	285589	1
Bombastus	Hydrophilic cream, non-ionic...	286325	1
Bombastus	Anionic hydrophilic cream DAB	287435	1
Bombastus	Base cream, hydrophobic DAC	289717	1
Apomix/Phönix	Anionic hydrophilic cream SR...	28A040815	1
Bombastus	Hydrophilic cream, non-ionic...	291387	1
Bombastus	Anionic hydrophilic cream DAB	291655	1
Bombastus	Hydrophilic cream, non-ionic...	292452	1
Bombastus	Hydrophilic cream, non-ionic...	292739	1
AHD	Anionic hydrophilic cream SR...	292976	1
AHD	Anionic hydrophilic cream SR...	292977	1
Bombastus	Anionic hydrophilic cream DAB	293358	1
AHD	Anionic hydrophilic cream SR...	296409	1
Bombastus	Anionic hydrophilic cream SR...	296410	2
Bombastus	Anionic hydrophilic cream SR...	297912	1
Bombastus	Anionic hydrophilic cream SR...	297910	1

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Supplier	Substance	Batch	Spectra
Bombastus	Anionic hydrophilic cream SR...	299254	2
Bombastus	Anionic hydrophilic cream SR...	29926	1
Bombastus	Anionic hydrophilic cream SR...	300950	2
Bombastus	Anionic hydrophilic cream SR...	300954	1
Bombastus	Anionic hydrophilic cream SR...	3213I-03327	1
Fagron	Hydrophilic cream, non-ionic...	3713U-03195	1
Apomix/Phönix	Anionic hydrophilic cream SR...	38A171115	1
AMH Niemann / apomix	Hydrophilic cream, non-ionic...	43a140714	1
Pharmachem/AHD	Base cream, hydrophobic DAC	110413	2
Sanacorp	Base cream, hydrophobic DAC	13085701	2
Caelo	Base cream, hydrophobic DAC	13274902	1
Sanacorp	Base cream, hydrophobic DAC	13175902	2
Sanacorp	Base cream, hydrophobic DAC	13275301	2
Euro OTC	Base cream, hydrophobic DAC		1
Pharmachem/AHD	Base cream, hydrophobic DAC	230713	1
Pharmachem/Phoenix	Base cream, hydrophobic DAC	240113	1
Pharmachem/AHD	Base cream, hydrophobic DAC	261112	1
Pharmachem/AHD	Base cream, hydrophobic DAC	26112	1
Gehe	Anionic hydrophilic cream DAB	262935	1
Bombastus	Hydrophilic cream, non-ionic...	265335	1
Bombastus	Anionic hydrophilic cream SR...	269230	1
Bombastus	Anionic hydrophilic cream SR...	266051	1
Bombastus	Hydrophilic cream, non-ionic...	268354	1
Bombastus	Anionic hydrophilic cream SR...	263823	1
Bombastus	Anionic hydrophilic cream DAB	269441	1
Fiebig	Anionic hydrophilic cream DAB	269445	1
Caelo	Anionic hydrophilic cream DAB	270943	2
Bombastus	Anionic hydrophilic cream DAB	271014	2
Gehe	Anionic hydrophilic cream SR...	271701	1
Gehe	Hydrophilic cream, non-ionic...	274216	1
Holdermann	Hydrophilic cream, non-ionic...	1B140113	1
apomix	Anionic hydrophilic cream SR...	5A300113	1
Caelo	Anionic hydrophilic cream DAB	11253201	1
Caelo	Anionic hydrophilic cream DAB	11326601	1
Anzag	Anionic hydrophilic cream DAB	12204601	2
Anzag	Anionic hydrophilic cream DAB	12218501	1
Sanacorp	Anionic hydrophilic cream DAB	12314401	1
Caelo	Anionic hydrophilic cream DAB	12245801	2
Caelo	Anionic hydrophilic cream DAB	1231401	1
Caelo	Anionic hydrophilic cream DAB	12314404	1
Caelo	Anionic hydrophilic cream wi...	13072401	6
Sanacorp	Anionic hydrophilic cream DAB	13154301	1
Caelo	Anionic hydrophilic cream DAB	13154301	5
Caelo	Anionic hydrophilic cream DAB	13167501-3423310192	1
Caelo	Anionic hydrophilic cream DAB	13167501-3439311151	1
Caelo	Anionic hydrophilic cream DAB	13167801	2
Caelo	Anionic hydrophilic cream DAB	13169201	4
Sanacorp	Anionic hydrophilic cream DAB	13168701	1
Caelo	Anionic hydrophilic cream wi...	13244402	9
Caelo	Anionic hydrophilic cream wi...	13244401-3471312131	1
Caelo	Anionic hydrophilic cream DAB	13280201-3452311172	1
Caelo	Anionic hydrophilic cream DAB	13312901	4
Caelo	Anionic hydrophilic cream DAB	13346101	4
Sanacorp	Anionic hydrophilic cream DAB	13313201	1
Caelo	Anionic hydrophilic cream DAB	13364301	3
Caelo	Anionic hydrophilic cream wi...	14030401	9
Bombastus	Anionic hydrophilic cream DAB	270711	1
Caelo	Anionic hydrophilic cream DAB	13409501	2
Anzag	Anionic hydrophilic cream DAB	271710	1
Bombastus	Anionic hydrophilic cream SR...	272513	1

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Supplier	Substance	Batch	Spectra
Bombastus	Hydrophilic cream, non-ionic...	274102	1
Sanacorp	Anionic hydrophilic cream SR...	274505	1
Gehe	Anionic hydrophilic cream DAB	274765	1
Bombastus	Anionic hydrophilic cream DAB	276316	1
Caelo	Anionic hydrophilic cream DAB	276409	1
Caelo	Anionic hydrophilic cream DAB	276319	1
Bombastus	Anionic hydrophilic cream DAB	277292	1
Sanacorp	Anionic hydrophilic cream SR...	277566	1
Sanacorp	Anionic hydrophilic cream SR...	277569	1
Bombastus	Anionic hydrophilic cream DAB	278849	1
Bombastus	Hydrophilic cream, non-ionic...	278027	1
EUro/AHD	Hydrophilic cream, non-ionic...	277577	1
Gehe	Anionic hydrophilic cream DAB	279057	1
Sanacorp	Anionic hydrophilic cream SR...	279202	1
Bomba/AHD	Anionic hydrophilic cream DAB	280410	1
Bombastus	Anionic hydrophilic cream SR...	279202	1
Bombastus	Anionic hydrophilic cream DAB	280416	1
Sanacorp	Anionic hydrophilic cream SR...	281742	1
Sanacorp	Anionic hydrophilic cream SR...	281809	1
Bombastus	Anionic hydrophilic cream DAB	281998	1
Bombastus	Anionic hydrophilic cream DAB	282111	2
Wolff/AHD	Anionic hydrophilic cream DAB	282107	1
Bombastus	Hydrophilic cream, non-ionic...	286838	1
Gehe	Anionic hydrophilic cream DAB	288653	1
Gehe	Hydrophilic cream, non-ionic...	288882	1
EUro/AHD	Hydrophilic cream, non-ionic...	34A240713	1
Apomix	Hydrophilic cream, non-ionic...	30B261112	1
Gehe	Anionic hydrophilic cream DAB	290080	1
Caelo	Anionic hydrophilic cream DAB	4051506	1
Caelo	Anionic hydrophilic cream DAB	6061501	1
Caelo	Anionic hydrophilic cream DAB	5031508	1
Caelo	Anionic hydrophilic cream DAB	9041505	1
Caelo	Anionic hydrophilic cream DAB	104/AKD2	1
Sanacorp	Anionic hydrophilic cream DAB	104/AKD3	1
Caelo	Anionic hydrophilic cream DAB	12081405	1
Caelo	Anionic hydrophilic cream wi...	12221003	3
Caelo	Anionic hydrophilic cream wi...	13172202	6
Caelo	Anionic hydrophilic cream DAB	13314302	3
Caelo	Anionic hydrophilic cream DAB	13314701	1
Caelo	Anionic hydrophilic cream DAB	133312901	1
Caelo	Anionic hydrophilic cream wi...	13343301	10
Caelo	Anionic hydrophilic cream wi...	13343401	15
Noweda	Anionic hydrophilic cream wi...	13343402	1
Caelo	Anionic hydrophilic cream wi...	13343402	6
Sanacorp	Anionic hydrophilic cream wi...	13343501	3
Caelo	Anionic hydrophilic cream wi...	13343501	5
Caelo	Anionic hydrophilic cream DAB	13346601	5
Caelo	Anionic hydrophilic cream DAB	13363301	5
Alliance Healthcare	Anionic hydrophilic cream DAB	13363401	1
Sanacorp	Anionic hydrophilic cream DAB	13364001	2
Cealo/Sanacorp	Anionic hydrophilic cream DAB	13364201	1
Caelo	Anionic hydrophilic cream DAB	13364201	2
Gehe am 21.02.14	Anionic hydrophilic cream DAB	13364401	1
Caelo	Anionic hydrophilic cream DAB	14016602	2
Fagron	Anionic hydrophilic cream DAB	14016602	1
Caelo	Anionic hydrophilic cream DAB	14016801	5
Caelo	Anionic hydrophilic cream DAB	14017001	2
Caelo	Anionic hydrophilic cream wi...	14030501	4
Phoenix	Anionic hydrophilic cream wi...	14030601	5
Caelo	Anionic hydrophilic cream wi...	14030701	25

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Supplier	Substance	Batch	Spectra
Euro OTC	Anionic hydrophilic cream wi...	14030701	1
Bombastus	Anionic hydrophilic cream wi...	14030701	1
Caelo	Anionic hydrophilic cream wi...	14030702	4
Phoenix	Anionic hydrophilic cream wi...	14030702	1
Caelo	Anionic hydrophilic cream DAB	14042301	1
Großhandel	Anionic hydrophilic cream DAB	14042401	1
Caelo	Anionic hydrophilic cream DAB	14042401	1
Caelo	Anionic hydrophilic cream DAB	14042501	1
Caelo	Anionic hydrophilic cream DAB	14042601	2
PHOENIX 22.05.2014	Anionic hydrophilic cream DAB	14061801	1
GEHE 22.03.2014	Anionic hydrophilic cream DAB	14062301	1
Caelo	Anionic hydrophilic cream DAB	14062501	5
Caesar & Loretz GmbH	Anionic hydrophilic cream DAB	14062401	1
Gehe	Anionic hydrophilic cream DAB	14062501	1
Gehe 01.08.14	Anionic hydrophilic cream DAB	14062501	1
Noweda	Anionic hydrophilic cream DAB	14062701	1
Caelo	Anionic hydrophilic cream DAB	14070801	1
Caelo	Anionic hydrophilic cream wi...	141146101	1
Bombastus	Anionic hydrophilic cream DAB	14118301	3
Phoenix	Anionic hydrophilic cream DAB	14118201	1
ahd/lamotte	Anionic hydrophilic cream DAB	14118401	1
Caelo	Anionic hydrophilic cream DAB	14138801	4
Caelo	Anionic hydrophilic cream DAB	14138902	3
Caelo	Anionic hydrophilic cream DAB	14138901	1
Phoenix 11.07.2014	Anionic hydrophilic cream DAB	14139001	2
Caesar & Loretz	Anionic hydrophilic cream DAB	14144301	1
AHDE 12.09.2014	Anionic hydrophilic cream DAB	14144301	1
Caelo	Anionic hydrophilic cream DAB	14144401	6
Caelo	Anionic hydrophilic cream DAB	14144501	3
Phoenix	Anionic hydrophilic cream wi...	14146001	2
Caelo	Anionic hydrophilic cream wi...	14146002	11
Caelo	Anionic hydrophilic cream wi...	14146003	4
Caelo	Anionic hydrophilic cream DAB	141460201	1
Caelo	Anionic hydrophilic cream wi...	14146101	7
Caelo	Anionic hydrophilic cream DAB	14146201	4
Caelo	Anionic hydrophilic cream DAB	14146501	2
Caelo	Anionic hydrophilic cream DAB	14146601	3
Caelo	Anionic hydrophilic cream DAB	1418101	2
Caelo	Anionic hydrophilic cream DAB	1415034401	1
Caelo	Anionic hydrophilic cream wi...	1416101	1
Caelo	Anionic hydrophilic cream DAB	14185201	4
Caelo	Anionic hydrophilic cream DAB	14185301	7
Caelo	Anionic hydrophilic cream DAB	14185401	4
Caelo	Anionic hydrophilic cream DAB	14185601	5
Caelo	Anionic hydrophilic cream DAB	14185702	1
Caesar & Loretz GmbH	Anionic hydrophilic cream DAB	14185801	1
Caelo	Anionic hydrophilic cream DAB	14185901	4
Caelo	Anionic hydrophilic cream DAB	14186001	2
Caelo	Anionic hydrophilic cream DAB	1418601	1
Sanacorp	Anionic hydrophilic cream DAB	14186702	1
Sanacorp	Anionic hydrophilic cream DAB	142/AKD52	1
Caelo	Anionic hydrophilic cream wi...	14214101	3
Caelo	Anionic hydrophilic cream wi...	14214201	1
Caelo	Anionic hydrophilic cream wi...	14214202	4
Phönix	Anionic hydrophilic cream wi...	14214202	2
Sanacorp	Anionic hydrophilic cream wi...	14214301	7
Caesar & Loretz GmbH	Anionic hydrophilic cream DAB	14232801	1
Caelo	Anionic hydrophilic cream DAB	14232801	2
Caelo	Anionic hydrophilic cream DAB	14232901	4
Caelo	Anionic hydrophilic cream DAB	142331001	1

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Supplier	Substance	Batch	Spectra
Alliance health	Anionic hydrophilic cream DAB	14233001	1
sanacorp	Anionic hydrophilic cream DAB	14233101	1
Alliance21.01.15	Anionic hydrophilic cream DAB	14233101	1
Phönix	Anionic hydrophilic cream DAB	14233401	1
Caelo	Anionic hydrophilic cream DAB	14233501	1
Caelo	Anionic hydrophilic cream wi...	1424202	1
Caelo	Anionic hydrophilic cream DAB	14255401	1
DAB 2008	Anionic hydrophilic cream DAB	14264001	1
AHD 05.03.15 3,33	Anionic hydrophilic cream DAB	14264001	1
Hedinger/Noweda	Anionic hydrophilic cream DAB	14264001	1
Phönix	Anionic hydrophilic cream DAB	14264301	1
Caelo	Anionic hydrophilic cream DAB	14264301	2
Sanacorp	Anionic hydrophilic cream DAB	14285601	1
Caelo	Anionic hydrophilic cream DAB	14285701	1
Caelo	Anionic hydrophilic cream DAB	14294501	1
Caelo	Anionic hydrophilic cream DAB	14294301	1
Caelo	Anionic hydrophilic cream DAB	14294601	1
Caelo	Anionic hydrophilic cream DAB	14294701	2
Caelo	Anionic hydrophilic cream DAB	14294801	2
Caelo	Anionic hydrophilic cream DAB	14295201	2
Caelo	Anionic hydrophilic cream DAB	14295101	1
Caelo	Anionic hydrophilic cream wi...	14334301	15
Sanacorp	Anionic hydrophilic cream wi...	14334401	1
Caelo	Anionic hydrophilic cream wi...	14334501	15
Caelo	Anionic hydrophilic cream wi...	14334502	5
sanacorp	Anionic hydrophilic cream DAB	14341601	1
Caelo	Anionic hydrophilic cream DAB	14341701	6
Caelo	Anionic hydrophilic cream DAB	14342101	5
Bombastus	Anionic hydrophilic cream DAB	14342501	2
Caelo	Anionic hydrophilic cream DAB	14342601	1
Caelo	Anionic hydrophilic cream DAB	14342901	2
Caesar & Loretz GmbH	Anionic hydrophilic cream DAB	15027301	1
Sanacorp	Anionic hydrophilic cream DAB	15034401	1
caesar&loretz,Phönix	Anionic hydrophilic cream DAB	15034301	1
Caelo	Anionic hydrophilic cream DAB	15034501	2
Caelo	Anionic hydrophilic cream wi...	15048301	12
Caelo	Anionic hydrophilic cream wi...	15048502	9
Caelo	Anionic hydrophilic cream wi...	1512901	1
Caelo	Anionic hydrophilic cream wi...	15132801	5
Caelo	Anionic hydrophilic cream wi...	15132901	4
Caelo	Anionic hydrophilic cream wi...	1513301	3
Caelo	Anionic hydrophilic cream DAB	15199901	4
Caelo	Anionic hydrophilic cream DAB	15200202	1
Caelo	Anionic hydrophilic cream DAB	15200301	4
Caelo	Anionic hydrophilic cream DAB	15200401	1
Cealo/Anzag	Anionic hydrophilic cream DAB	15200401	1
Caesar&loretz,Anzag	Anionic hydrophilic cream DAB	15258901	1
Caelo	Anionic hydrophilic cream DAB	15267001	1
Caelo	Anionic hydrophilic cream DAB	15267701	1
Caelo	Anionic hydrophilic cream wi...	15272901	1
Caelo	Anionic hydrophilic cream wi...	15273101	9
Caelo	Anionic hydrophilic cream wi...	15273201	9
Rondell Apotheke	Anionic hydrophilic cream wi...	15273301	1
Caelo	Anionic hydrophilic cream DAB	15315501	2
Fischer/Gehe	Anionic hydrophilic cream DAB	15315601	1
Caelo	Anionic hydrophilic cream DAB	15319101	1
Caelo	Anionic hydrophilic cream DAB	15319201	3
Caelo	Anionic hydrophilic cream DAB	1535101	1
Caelo	Anionic hydrophilic cream DAB	153552901	1
Caelo	Anionic hydrophilic cream DAB	15357101	1

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Supplier	Substance	Batch	Spectra
Caelo	Anionic hydrophilic cream DAB	15357201	1
Caelo	Anionic hydrophilic cream DAB	15357501	2
Caelo	Anionic hydrophilic cream DAB	15396901	1
Caelo	Anionic hydrophilic cream DAB	15397101	1
Caelo	Anionic hydrophilic cream DAB	15400501	2
Noweda	Anionic hydrophilic cream DAB	15400501	1
Caesar & Loretz GmbH	Anionic hydrophilic cream DAB	15400601	1
Caelo	Anionic hydrophilic cream DAB	15400901	1
Sanacorp 21,01.16	Anionic hydrophilic cream DAB	15400901	1
Sanacorp	Anionic hydrophilic cream DAB	15401201	1
Caelo	Anionic hydrophilic cream DAB	15401302	4
Caelo	Anionic hydrophilic cream DAB	15401501	1
Caelo	Anionic hydrophilic cream DAB	15401701	2
Caelo	Anionic hydrophilic cream wi...	15405301	6
Caeol/AHD	Anionic hydrophilic cream wi...	15405301	1
Caelo	Anionic hydrophilic cream DAB	15428201	1
Caelo	Anionic hydrophilic cream DAB	15428301	2
Caelo	Anionic hydrophilic cream DAB	15431801	2
Caelo	Anionic hydrophilic cream DAB	15431901	2
Caelo	Anionic hydrophilic cream wi...	1548301	2
Caelo	Anionic hydrophilic cream DAB	16046501	1
Gehe	Anionic hydrophilic cream wi...	16067301	1
Caelo	Anionic hydrophilic cream wi...	16067401	1
Caelo	Anionic hydrophilic cream DAB	16071506	1
Caelo	Anionic hydrophilic cream DAB	161431	1
Caelo	Anionic hydrophilic cream wi...	20071504	1
Caelo	Anionic hydrophilic cream wi...	2114M25401	1
Caelo	Anionic hydrophilic cream DAB	2111401	1
Caelo	Anionic hydrophilic cream DAB	2414E2540	1
Sanacorp	Anionic hydrophilic cream wi...	24AKD1	1
Caelo	Anionic hydrophilic cream wi...	2514U25401	1
Caelo	Anionic hydrophilic cream wi...	27031504	1
Caelo	Anionic hydrophilic cream DAB	27041512	1
Caesar & Loretz GmbH Hi...	Anionic hydrophilic cream DAB	280291	1
Bombastus	Anionic hydrophilic cream DAB	283477	1
Bombastus	Anionic hydrophilic cream DAB	288575	1
Bombastus	Anionic hydrophilic cream DAB	288720	1
Bombastus	Anionic hydrophilic cream DAB	290075	1
Caelo	Anionic hydrophilic cream DAB	290145	1
Bombastus	Anionic hydrophilic cream DAB	290218	2
Bombastus	Anionic hydrophilic cream DAB	291825	1
Bombastus	Anionic hydrophilic cream DAB	294643	2
Bombastus	Anionic hydrophilic cream DAB	294644	2
Bombastus	Anionic hydrophilic cream DAB	294646	1
Bombastus	Anionic hydrophilic cream DAB	295399	1
Bombastus	Anionic hydrophilic cream DAB	295401	1
Bombastus	Anionic hydrophilic cream DAB	295404	1
Bombastus	Anionic hydrophilic cream DAB	296700	1
Bombastus	Anionic hydrophilic cream DAB	296702	1
Bombastus	Anionic hydrophilic cream DAB	296705	1
Bombastus	Anionic hydrophilic cream DAB	296781	1
Bombastus	Anionic hydrophilic cream DAB	297680	2
Caelo	Anionic hydrophilic cream DAB	300353	1
Caelo	Anionic hydrophilic cream DAB	30091403	1
Caelo	Anionic hydrophilic cream wi...	32/AKD2	1
Sanacorp	Anionic hydrophilic cream wi...	39/AKD4	1
Sanacorp	Anionic hydrophilic cream wi...	41/AKD6	1
Sanacorp	Anionic hydrophilic cream wi...		1
Caesar & Loretz GmbH Hi...	Anionic hydrophilic cream wi...	B1334301	1
Caelo	Anionic hydrophilic cream wi...	CHB13343401	1

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Supplier	Substance	Batch	Spectra
Caelo	Anionic hydrophilic cream wi...	112210016	1
Caelo	Anionic hydrophilic cream DAB	112212540	1
Phönix	Anionic hydrophilic cream DAB	13265602	1
Caelo	Anionic hydrophilic cream DAB	314Q2540	1
eigene Herstellung	Anionic hydrophilic cream DAB	2/270114	1
Caelo	Anionic hydrophilic cream DAB	6021405	1
Caelo	Anionic hydrophilic cream DAB	6021406	1
Caelo	Anionic hydrophilic cream wi...	7011403	1
Caelo	Anionic hydrophilic cream DAB	714M2540	1
Caelo	Anionic hydrophilic cream DAB	8051301	1
Caelo	Anionic hydrophilic cream DAB	8111301	1
Caelo	Anionic hydrophilic cream SR...	9101202	1
Caelo	Anionic hydrophilic cream wi...	9771644	1
eigene Herstellung	Anionic hydrophilic cream DAB	100214-4	1
Caelo	Anionic hydrophilic cream DAB	1108053-02	1
Caelo	Anionic hydrophilic cream SR...	1109212540	1
Caelo	Anionic hydrophilic cream DAB	1114U2540	1
Gehe	Anionic hydrophilic cream DAB	11219901	1
noweda	Anionic hydrophilic cream DAB	11238910	1
Caelo	Anionic hydrophilic cream DAB	113313001	2
Caelo	Anionic hydrophilic cream DAB	12010501	1
Caelo	Anionic hydrophilic cream DAB	12010601	1
Caelo	Anionic hydrophilic cream DAB	12026001	1
Caelo	Anionic hydrophilic cream DAB	12084101	3
Caelo	Anionic hydrophilic cream DAB	12100101	1
Caesar & Loretz GmbH, 4...	Anionic hydrophilic cream DAB	12100601	1
Caelo	Anionic hydrophilic cream DAB	12101101	1
Caesar & Loretz GmbH	Anionic hydrophilic cream DAB	12101101	1
Caelo	Anionic hydrophilic cream DAB	12101302	1
Caelo	Anionic hydrophilic cream wi...	1213M-07009	1
Caelo	Anionic hydrophilic cream DAB	1218501	1
Noweda	Anionic hydrophilic cream DAB	1218701	1
Caelo	Anionic hydrophilic cream DAB	12187801	2
Caelo	Anionic hydrophilic cream DAB	12188001	1
Caelo	Anionic hydrophilic cream DAB	12188101	1
Caelo	Anionic hydrophilic cream DAB	12195301	1
Noweda	Anionic hydrophilic cream DAB	12204701	1
Caelo	Anionic hydrophilic cream wi...	12216501	1
Caelo	Anionic hydrophilic cream DAB	12217801	5
Noweda	Anionic hydrophilic cream DAB	12217801	1
Caelo	Anionic hydrophilic cream DAB	12217901	2
Caelo	Anionic hydrophilic cream DAB	12218001	2
Phönix 12.10.2012	Anionic hydrophilic cream DAB	12218201	1
Caelo	Anionic hydrophilic cream DAB	12218201	2
Caelo	Anionic hydrophilic cream DAB	12218701	1
Caelo	Anionic hydrophilic cream DAB	12218801	3
Caelo	Anionic hydrophilic cream wi...	12221002	5
vdl	Anionic hydrophilic cream wi...	12221002	1
Caelo	Anionic hydrophilic cream wi...	1222102	1
Caelo	Anionic hydrophilic cream DAB	12245503	1
Sanacorp	Anionic hydrophilic cream DAB	12264401	1
Caelo	Anionic hydrophilic cream DAB	12264501	4
Caelo	Anionic hydrophilic cream DAB	12264401	1
Hedinger	Anionic hydrophilic cream DAB	12264501	1
Caelo	Anionic hydrophilic cream DAB	12264502	1
Caelo	Anionic hydrophilic cream DAB	12264701	2
Caelo	Anionic hydrophilic cream DAB	12264901	1
Caelo	Anionic hydrophilic cream DAB	12265001	2
Gehe	Anionic hydrophilic cream DAB	12265001	1
Caelo	Anionic hydrophilic cream DAB	12265101	1

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Supplier	Substance	Batch	Spectra
Fagron	Anionic hydrophilic cream DAB	12265501	1
Caelo	Anionic hydrophilic cream DAB	12265901	1
Phoenix 25.01.2013	Anionic hydrophilic cream DAB	12265901	1
Caelo	Anionic hydrophilic cream wi...	12301301	2
Caelo	Anionic hydrophilic cream wi...	12283001	1
GEHE	Anionic hydrophilic cream wi...	12301302	1
Caelo	Anionic hydrophilic cream wi...	12301302	5
Fagron	Anionic hydrophilic cream DAB	12313202	1
Caelo	Anionic hydrophilic cream DAB	12313301	4
Gehe	Anionic hydrophilic cream DAB	12313401	1
Caelo	Anionic hydrophilic cream DAB	12313401	1
Caelo	Anionic hydrophilic cream DAB	12313501	5
Caesar & Loretz GmbH	Anionic hydrophilic cream DAB	12313501	1
Post-Apotheke	Anionic hydrophilic cream DAB	12313701	1
Phoenix 26.03.13	Anionic hydrophilic cream DAB	12313901	1
Caelo	Anionic hydrophilic cream DAB	12314201	4
Noweda	Anionic hydrophilic cream DAB	12314301	1
Großhandel	Anionic hydrophilic cream DAB	12314201	1
Großhandel	Anionic hydrophilic cream DAB	12314501	1
Caelo	Anionic hydrophilic cream DAB	12314501	2
Phönix 10.04.2013	Anionic hydrophilic cream DAB	12314501	1
Phönix	Anionic hydrophilic cream DAB	1231451	1
Großhandel	Anionic hydrophilic cream DAB	12314901	1
Caelo	Anionic hydrophilic cream DAB	1234301	1
Caelo	Anionic hydrophilic cream wi...	12344401	1
Caelo	Anionic hydrophilic cream DAB	1234569	1
Caelo	Anionic hydrophilic cream wi...	12352701	5
Caelo	Anionic hydrophilic cream wi...	12352702	4
Caesar & Loretz GmbH, 4...	Anionic hydrophilic cream wi...	12352702	1
Caelo	Anionic hydrophilic cream wi...	12352703	2
Caelo	Anionic hydrophilic cream DAB	13035902	4
Noweda	Anionic hydrophilic cream DAB	13035902	1
Phönix	Anionic hydrophilic cream DAB	13036001	1
Caelo	Anionic hydrophilic cream DAB	13036302	1
Phoenix	Anionic hydrophilic cream DAB	13038201	1
Gehe	Anionic hydrophilic cream DAB	13038201	1
Caelo	Anionic hydrophilic cream DAB	13071304	1
Caelo	Anionic hydrophilic cream wi...	13072301	2
Caelo	Anionic hydrophilic cream wi...	13072302	10
Caesar & Loretz GmbH, 4...	Anionic hydrophilic cream wi...	13072302	3
Noweda	Anionic hydrophilic cream wi...	13072302	1
Caelo	Anionic hydrophilic cream wi...	13072303	3
GEHE	Anionic hydrophilic cream wi...	13072303	1
Caelo	Anionic hydrophilic cream wi...	130723301	1
noweda	Anionic hydrophilic cream wi...	13072401	1
Noweda	Anionic hydrophilic cream wi...	13072401	1
PHÖNIX 06.06.2013	Anionic hydrophilic cream wi...	13072401	1
Caelo	Anionic hydrophilic cream SR...	1310212540	1
Caelo	Anionic hydrophilic cream wi...	13125901	8
Caesar & Loretz GmbH, 4...	Anionic hydrophilic cream wi...	13125901	2
Caelo	Anionic hydrophilic cream wi...	13125902	3
Caelo	Anionic hydrophilic cream wi...	13125903	1
Caesar&lorenz,Phoenix	Anionic hydrophilic cream DAB	13128701	1
Sanacorp	Anionic hydrophilic cream DAB	13154101	1
Gehe	Anionic hydrophilic cream DAB	13154201	2
Caelo	Anionic hydrophilic cream DAB	13154401	1
Cealo	Anionic hydrophilic cream wi...	13165001	1
Großhandel	Anionic hydrophilic cream DAB	13165101	1
Gehe	Anionic hydrophilic cream DAB	13165701	1
Noweda	Anionic hydrophilic cream DAB	13167401	1

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Supplier	Substance	Batch	Spectra
Caelo	Anionic hydrophilic cream DAB	13167401	1
Caelo	Anionic hydrophilic cream DAB	13167701	2
Caelo	Anionic hydrophilic cream DAB	13168001	6
Sanacorp	Anionic hydrophilic cream DAB	13168001	1
Caelo	Anionic hydrophilic cream DAB	13168301	5
Caelo	Anionic hydrophilic cream DAB	13168501	9
Noweda	Anionic hydrophilic cream DAB	13168601	1
Caelo	Anionic hydrophilic cream DAB	13168701	5
Caelo	Anionic hydrophilic cream DAB	13169101	4
Großhandel	Anionic hydrophilic cream DAB	13169201	1
Caelo	Anionic hydrophilic cream wi...	13172201	1
Phönix	Anionic hydrophilic cream wi...	13172203	1
Caelo	Anionic hydrophilic cream wi...	13172203	4
Noweda	Anionic hydrophilic cream wi...	13172203	1
Caelo	Anionic hydrophilic cream wi...	1324401	1
Phönix/gepepharm	Anionic hydrophilic cream wi...	13244201	2
Caelo	Anionic hydrophilic cream wi...	1324402	1
Caelo	Anionic hydrophilic cream wi...	13244201	8
Caesar & Loretz GmbH, 4...	Anionic hydrophilic cream wi...	13244201	1
Caelo	Anionic hydrophilic cream wi...	13244301	4
Caelo	Anionic hydrophilic cream wi...	13244302	2
Caesar & Loretz GmbH, 4...	Anionic hydrophilic cream wi...	13244401	1
Caelo	Anionic hydrophilic cream wi...	13244401	13
Gehe	Anionic hydrophilic cream wi...	13244401	1
Caelo	Anionic hydrophilic cream DAB	13265501	5
Phoenix 26.11.13	Anionic hydrophilic cream DAB	13265501	1
Caelo	Anionic hydrophilic cream DAB	13265701	1
Noweda	Anionic hydrophilic cream DAB	13270801	1
Caelo	Anionic hydrophilic cream DAB	13271001	3
Cealo/Sanacorp	Anionic hydrophilic cream DAB	13275501	1
Caelo	Anionic hydrophilic cream DAB	13275501	1
Caelo	Anionic hydrophilic cream DAB	13275701	1
Caelo	Anionic hydrophilic cream DAB	13280001	1
Noweda	Anionic hydrophilic cream DAB	13280101	1
Sanacorp	Anionic hydrophilic cream DAB	13280201	1
Gehe	Anionic hydrophilic cream DAB	13280201	1
Caelo	Anionic hydrophilic cream DAB	13310001	1
Großhandel	Anionic hydrophilic cream DAB	13312901	1
Sanacorp	Anionic hydrophilic cream DAB	13313101	1
AHD, 31.10.2013	Anionic hydrophilic cream DAB	13313201	1
Phönix 11.11.2014	Anionic hydrophilic cream DAB	13313301	1
Caesar & Loretz	Anionic hydrophilic cream DAB	13313301	1
Caelo	Anionic hydrophilic cream DAB	13313401	4
Großhandel	Anionic hydrophilic cream DAB	13313601	1
Caelo	Anionic hydrophilic cream DAB	13314601	2
Phoenix	Anionic hydrophilic cream DAB	13314901	1
Caelo	Anionic hydrophilic cream wi...	1334302	1
Noweda	Anionic hydrophilic cream wi...	13343301	1
Caelo	Anionic hydrophilic cream DAB	13346001	4
Caelo	Anionic hydrophilic cream wi...	13344301	1
Phoenix 24.01.2014	Anionic hydrophilic cream DAB	13346101	1
Phönix	Anionic hydrophilic cream DAB	13346301	1
Großhandel	Anionic hydrophilic cream DAB	13346401	1
Caesar & Loretz GmbH Hi...	Anionic hydrophilic cream DAB	13346401	1
Caelo	Anionic hydrophilic cream DAB	13346401	1
Caelo	Anionic hydrophilic cream DAB	13346501	3
Caelo	Anionic hydrophilic cream DAB	13346701	1
Großhandel	Anionic hydrophilic cream DAB	13346701	1
Caelo	Anionic hydrophilic cream DAB	13363401	1
Caesar&lorenz,Phoenix	Anionic hydrophilic cream DAB	13363601	1

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Supplier	Substance	Batch	Spectra
Phoenix	Anionic hydrophilic cream DAB	13364201	1
Caesar & Loretz GmbH	Anionic hydrophilic cream DAB	13409401	1
Caelo	Anionic hydrophilic cream DAB	1368001	1
Großhandel	Anionic hydrophilic cream DAB	1369201	1
Phoenix	Anionic hydrophilic cream DAB	14016602	1
Caesar&loretz,Phoenix	Anionic hydrophilic cream wi. . .	14030701	1
Gehe	Anionic hydrophilic cream DAB	14042201	1
Caelo	Anionic hydrophilic cream DAB	14042201	1
Caesar&loretz,Phoenix	Anionic hydrophilic cream DAB	14118201	1
Caesar&loretz,Phoenix	Anionic hydrophilic cream DAB	14139001	1
Phoenix	Anionic hydrophilic cream DAB	14139001	1
Caesar&loretz,phönix	Anionic hydrophilic cream DAB	14186702	1
Caesar&loretz,Phoenix	Anionic hydrophilic cream DAB	14285601	1
Caelo	Anionic hydrophilic cream DAB	142/AKD51	1
Caesar&loretz,Phoenix	Anionic hydrophilic cream DAB	14294801	1
Caesar&loretz,Phoenix	Anionic hydrophilic cream DAB	14233601	1
Caelo	Anionic hydrophilic cream DAB	1601312540	2
Caelo	Anionic hydrophilic cream wi. . .	18/AKD1511	1
Caelo	Anionic hydrophilic cream DAB	19101301	1
Caelo	Anionic hydrophilic cream DAB	20021311	1
Caelo	Anionic hydrophilic cream DAB	20301012-3	1
Caelo	Anionic hydrophilic cream DAB	22091202	1
Caelo	Anionic hydrophilic cream DAB	24021401	1
Caelo	Anionic hydrophilic cream SR. . .	21081201	1
Euro OTC	Anionic hydrophilic cream DAB	237563	1
Caelo	Anionic hydrophilic cream DAB	2413Q02540	1
Bombastus	Anionic hydrophilic cream DAB	273538	1
Bombastus	Anionic hydrophilic cream DAB	274600	1
Bombastus	Anionic hydrophilic cream DAB	274696	1
Anzag, 28.11.12	Anionic hydrophilic cream DAB	274696	1
Bombastus	Anionic hydrophilic cream DAB	274698	1
Phönix	Anionic hydrophilic cream DAB	276433	1
Bombastus	Anionic hydrophilic cream DAB	280288	2
Bombastus	Anionic hydrophilic cream DAB	280413	1
Bombastus	Anionic hydrophilic cream DAB	282107	1
Bombastus	Anionic hydrophilic cream DAB	283412	1
Caelo	Anionic hydrophilic cream wi. . .	2913M25401	1
Caelo	Anionic hydrophilic cream DAB	30081301	1
Caelo	Anionic hydrophilic cream wi. . .	3125902	1
Caelo	Anionic hydrophilic cream DAB	3313U-02540	1
Caelo	Anionic hydrophilic cream DAB	3413M-02540	1
Caelo	Anionic hydrophilic cream DAB	3713A02540	1
Caelo	Anionic hydrophilic cream DAB	3321	1
Caelo	Anionic hydrophilic cream DAB	4513E2540	1
Caelo	Anionic hydrophilic cream DAB	4513U2540	1
Caelo	Anionic hydrophilic cream wi. . .	Ch13125901	1
Caelo	Anionic hydrophilic cream DAB	Ch13128601	1
Caelo	Anionic hydrophilic cream DAB	CH13314001	1
Caelo	Anionic hydrophilic cream DAB	pzn01119720	1
Caelo	Anionic hydrophilic cream DAB	U-030513-1	1
Caelo	Anionic hydrophilic cream DAB	U-310513-1	1
Dr. Wolff	Wolff [®] basic half-fat cream	12081508	1
Dr. Wolff/Noweda	Wolff [®] basic half-fat cream	434360	4
Dr. Wolff	Wolff [®] basic half-fat cream	436750	3
Wolff/ Gehe	Wolff [®] basic half-fat cream	434360	1
Dr. August Wolff	Wolff [®] basic half-fat cream	434360	1
Wolff/Alliance	Wolff [®] basic half-fat cream	436750	1
Dr. Wolff	Wolff [®] basic half-fat cream	438160	1
Dr. Wolff / Kehr	Wolff [®] basic half-fat cream	438160	1
Dr. Wolff GmbH & Co.KG A. . .	Wolff [®] basic half-fat cream	438160	1

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Supplier	Substance	Batch	Spectra
A. Wolff/Kehr	Wolff [®] basic half-fat cream	438340	2
wolff GmbH/AHD 21.09.2015	Wolff [®] basic half-fat cream	438340	1
Wolff/Phoenix	Wolff [®] basic half-fat cream	4715E-03719	1
Wolff	Wolff [®] basic half-fat cream	501080	3
Dr. Wolff	Wolff [®] basic half-fat cream	501080	1
Wolff GmbH	Wolff [®] basic half-fat cream	501080	1
Dr. Wolff GmbH	Wolff [®] basic half-fat cream	501080	1
Sanacorp/Dr. Wolff	Wolff [®] basic half-fat cream	501082	1
Dr. Wolff	Wolff [®] basic half-fat cream	501082	1
Dr. Wolff	Wolff [®] basic half-fat cream	501470	1
Wolff/Phönix	Wolff [®] basic half-fat cream	501470	1
Dr. Wolff/Noweda	Wolff [®] basic half-fat cream	501082	1
Caelo	Wolff [®] basic half-fat cream	501470	3
Dr. Wolff/ Phoenix	Wolff [®] basic half-fat cream	501470	2
Wolff GmbH / Noweda	Wolff [®] basic half-fat cream	501470	1
Wolff/ Anzag	Wolff [®] basic half-fat cream	501470	1
Dr. Wolff / Gehe	Wolff [®] basic half-fat cream	501870	1
Wolff	Wolff [®] basic half-fat cream	506360	1
Dr. August Wolff GmbH	Wolff [®] basic half-fat cream	506360	1
Dr. Wolff	Wolff [®] basic half-fat cream	510400	1
Caelo	Wolff [®] basic half-fat cream	506361	1
Euro OTC	Wolff [®] basic half-fat cream	510400	1
Dr. Wolff	Wolff [®] basic half-fat cream	510400	1
Gehe/ Wolff	Wolff [®] basic half-fat cream	510400	1
Wolff/AHD	Wolff [®] basic half-fat cream	510621	1
Dr. Wolff/Phönix	Wolff [®] basic half-fat cream	510621	1
Dr. Wolff / Kehr	Wolff [®] basic half-fat cream	510621	1
Dr Wolff/Noweda	Wolff [®] basic half-fat cream	511420	3
Wolf	Wolff [®] basic half-fat cream	511420	1
Caelo	Wolff [®] basic half-fat cream	511420	2
Dr. August Wolff	Wolff [®] basic half-fat cream	511420	1
Dr. August Wolff GmbH	Wolff [®] basic half-fat cream	511420	2
Phoenix	Wolff [®] basic half-fat cream	511420	1
Wolff/Alliance	Wolff [®] basic half-fat cream	511420	1
Caelo	Wolff [®] basic half-fat cream	602050	1
Phoenix	Wolff [®] basic half-fat cream	602050	3
Dr. August Wolff GmbH	Wolff [®] basic half-fat cream	602050	2
Caelo	Wolff [®] basic half-fat cream	602290	1
AHD	Wolff [®] basic half-fat cream	602290	1
Dr. Wolff / Kehr	Wolff [®] basic half-fat cream	602290	1
Dr. Wolff / Kehr	Wolff [®] basic half-fat cream	605700	1
Caelo	Wolff [®] basic half-fat cream	606050	1
Dr Wolff/ Gehe	Wolff [®] basic half-fat cream	234791	1
Caelo	Wolff [®] basic half-fat cream	235200	1
Dr. Wolff	Wolff [®] basic half-fat cream	331551	2
Wolff/Gehe	Wolff [®] basic half-fat cream	236420	1
wolff/AHD	Wolff [®] basic half-fat cream	332040	10
Wolff/AHD	Wolff [®] basic half-fat cream	332040	5
Euro OTC	Wolff [®] basic half-fat cream	332040	4
Caelo	Wolff [®] basic half-fat cream	332040	6
Wolff	Wolff [®] basic half-fat cream	332040	5
Phönix Gotha	Wolff [®] basic half-fat cream	332040	2
Wolff GmbH/Sanacorp	Wolff [®] basic half-fat cream	333620	3
Dr. Wolff/Sanacorp	Wolff [®] basic half-fat cream	333620	1
Dr Wolff/ Gehe	Wolff [®] basic half-fat cream	333930	1
Phoenix/Wolff	Wolff [®] basic half-fat cream	333930	1
Dr. Wolff/Noweda	Wolff [®] basic half-fat cream	333930	2
Dr. Wolff	Wolff [®] basic half-fat cream	333930	3
Dr. Wolff	Wolff [®] basic half-fat cream	337260	3
Dr Wolff/ Sanacorp	Wolff [®] basic half-fat cream	339140	1

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Supplier	Substance	Batch	Spectra
Wolff GmbH/Sanacorp	Wolff [®] basic half-fat cream	339140	1
Dr. Wolff	Wolff [®] basic half-fat cream	339140	1
Anzag/ Dr. Wolff	Wolff [®] basic half-fat cream	339140	1
Cealo/Phönix	Wolff [®] basic half-fat cream	339140	1
Wolf/Phönix	Wolff [®] basic half-fat cream	430880	2
Wolff/Alliance	Wolff [®] basic half-fat cream	430880	1
Dr. Wolff/V.d.L.	Wolff [®] basic half-fat cream	430880	4
Wolff	Wolff [®] basic half-fat cream	430880	1
Hedinger/Noweda	Wolff [®] basic half-fat cream	430880	2
Wolff/ Phönix	Wolff [®] basic half-fat cream	430880	2
Dr. Wolff/ Gehe	Wolff [®] basic half-fat cream	430880	1
Dr. August Wolff	Wolff [®] basic half-fat cream	430880	1
Euro/Gehe	Wolff [®] basic half-fat cream	431050	1
Caelo	Wolff [®] basic half-fat cream	431050	1
wolff	Wolff [®] basic half-fat cream	431050	1
Gehe	Wolff [®] basic half-fat cream	431050	1
Dr. Wolff	Wolff [®] basic half-fat cream	431240	2
Caelo	Wolff [®] basic half-fat cream	431240	2
Wolff	Wolff [®] basic half-fat cream	431240	2
wolff/AHD	Wolff [®] basic half-fat cream	431240	1
Dr. Wolff	Wolff [®] basic half-fat cream	431240	1
wolff	Wolff [®] basic half-fat cream	431240	1
Dr. Wolff /Anzag	Wolff [®] basic half-fat cream	432611	1
Dr. Wolff GmbH & Co.KG A...	Wolff [®] basic half-fat cream	432611	1
Caelo	Wolff [®] basic half-fat cream	434360	2
Dr. Wolff/NOW	Wolff [®] basic half-fat cream	432611	1
Dr. Wolff/ Sanacorp	Wolff [®] basic half-fat cream	434360	1
Phoenix	Wolff [®] basic half-fat cream	434360	1
Dr. Wolff/NOW	Wolff [®] basic half-fat cream	434581	1
Dr. Wolff GmbH & Co.KG A...	Wolff [®] basic half-fat cream	434581	1
Dr. August Wolff	Wolff [®] basic half-fat cream	38800	1
Phönix Gotha	Wolff [®] basic half-fat cream	134990	1
Löwen City-Apotheke Bar...	Wolff [®] basic half-fat cream	230200	1
Wolff GmbH	Wolff [®] basic half-fat cream	230870	1
Dr. Wolff /Anzag	Wolff [®] basic half-fat cream	232593	1
Spirig/Anzag	Wolff [®] basic half-fat cream	234791	1
Dr. Wolff/Noweda	Wolff [®] basic half-fat cream	234791	2
Sanacorp	Wolff [®] basic half-fat cream	235200	2
Dr. Wolff/ Anzag	Wolff [®] basic half-fat cream	235200	1
DR. August Wolff GmbH	Wolff [®] basic half-fat cream	235200	1
Fagron	Wolff [®] basic half-fat cream	236320	3
Dr. Wolff	Wolff [®] basic half-fat cream	236320	1
Dr. Wolff	Wolff [®] basic half-fat cream	236420	1
Dr. Wolff	Wolff [®] basic half-fat cream	238490	2
Dr. Wolff	Wolff [®] basic half-fat cream	238560	5
Dr. Wolff	Wolff [®] basic half-fat cream	238560	2
Caelo	Wolff [®] basic half-fat cream	238560	1
Wolff GmbH	Wolff [®] basic half-fat cream	238560	1
Dr. Wolff/Gehe	Wolff [®] basic half-fat cream	238660	1
Phönix	Wolff [®] basic half-fat cream	238560	1
Dr. Wolff/Noweda	Wolff [®] basic half-fat cream	238660	1
Wolff/AHD	Wolff [®] basic half-fat cream	331551	8
Wolff	Wolff [®] basic half-fat cream	238660	1
Dr. Wolf	Wolff [®] basic half-fat cream	331551	1
Gehe	Wolff [®] basic half-fat cream	331551	2
Dr. Wolff	Wolff [®] basic half-fat cream	332040	1
Phönix	Wolff [®] basic half-fat cream	333620	2
Dr. Wolff/Sanacorp	Wolff [®] basic half-fat cream	333620	1
Dr. August Wolff	Wolff [®] basic half-fat cream	333620	1
Dr. Wolff	Wolff [®] basic half-fat cream	333620	5

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Supplier	Substance	Batch	Spectra
Caelo	Wolff [®] basic half-fat cream	333620	3
Dr. Wolff / Noweda	Wolff [®] basic half-fat cream	333930	1
Dr. Wolff	Wolff [®] basic half-fat cream	333930	2
Caelo	Wolff [®] basic half-fat cream	333930	1
Dr. August Wolff/Sanaco...	Wolff [®] basic half-fat cream	337260	1
Dr. Wolff	Wolff [®] basic half-fat cream	432611	1

- 52 455 spectra from 332 *Apo-Ident* customers from a total of 18 006 batches from a further 318 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 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 *Hydrophilic 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	2010	0	32 334
Type B	0	10 686	7	52 312
Type C	0	5653	333	52 333

The substance/substance group *Hydrophilic 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 % (> 99.9689 %)	100.0000 % (> 99.7015 %)
Type B	100.0000 % (> 99.9713 %)	99.9345 % (> 99.9065 %)
Type C	100.0000 % (> 99.6110 %)	94.4370 % (> 94.3869 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30631	30837	8.24	35.94
30758	31907	7.37	39.28
30769	30769	0.00	24.97
30837	30837	0.00	33.70
30880	31741	6.36	27.76
30895	31054	6.97	34.83
30931	31478	10.68	40.58
31002	31907	3.31	37.34
31008	31008	0.00	21.11
31039	31039	0.00	30.45
31040	31503	6.86	29.68
31042	31008	9.20	23.98
31054	31054	0.00	32.63
31086	30837	12.99	32.09
31188	31188	0.00	26.00
31231	31231	0.00	32.72
31241	31741	3.87	33.99
31440	31440	0.00	29.26
31450	32123	6.03	26.13
31470	31741	3.24	34.05
31477	31188	3.30	24.67
31478	31478	0.00	37.49
31487	30837	18.95	30.25
31500	31500	0.00	28.00
31503	31503	0.00	32.82
31516	31996	14.73	36.79
31537	31537	0.00	36.00
31565	31996	9.00	30.04
31568	30769	5.00	25.36
31591	31996	6.87	25.08
31593	31996	3.48	26.26
31599	31188	2.23	26.09
31600	31039	7.73	32.13
31644	31799	3.49	38.59
31661	31537	8.85	33.95
31741	31741	0.00	32.91
31799	31799	0.00	38.40
31906	31906	0.00	35.71
31907	31907	0.00	36.65
31962	31054	13.61	36.03
31996	31996	0.00	26.94
32022	32022	0.00	30.95
32039	32039	0.00	20.86
32052	32052	0.00	30.84
32123	32123	0.00	28.46
32132	32132	0.00	33.66
32142	32142	0.00	20.17
32303	31799	2.51	35.93
32346	31008	5.61	22.33
32435	32435	0.00	27.76

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Hydroxyethyl salicylate
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30638-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydroxyethyl salicylate; Hydroxyethyl salicylicum; Hydroxyethyl salicylas

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Hydroxyethyl salicylate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydroxyethyl sal...	12049001	30638	40	1402192
Caelo	Hydroxyethyl sal...	13285709	31339	40	20130918

Validation samples

A total of 156 379 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 *Hydroxyethyl salicylate*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Hydroxyethyl salicylate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydroxyethyl salicylate	16131002	32588	40
Caelo	Hydroxyethyl salicylate	16131009	33241	40

- 63 514 spectra from a total of 1475 batches from further 439 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 *Hydroxyethyl salicylate*.

Supplier	Substance	Batch	Spectra
Caelo	Hydroxyethyl salicylate	13285702	1
Caelo	Hydroxyethyl salicylate	2091302	1

- 58 439 spectra from 332 *Apo-Ident* customers from a total of 20 090 batches from a further 328 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 *Hydroxyethyl salicylate* 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 *Hydroxyethyl salicylate* 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	34 264
Type B	0	80	0	63 514
Type C	0	2	0	58 439

The substance/substance group *Hydroxyethyl salicylate* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.6008 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30638	30638	0.00	78.32
31339	30638	8.81	70.73

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Isopropyl alcohol 100%
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30759-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Isopropyl alcohol 100%; Alcohol isopropylicus 100%

Special notes

When selecting the *Isopropyl alcohol 100%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Isopropyl alcohol 100%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Isopropyl alcoho...	12321002	30759	40	20121102
Caelo	Isopropyl alcoho...	13249425	31232	40	20130726
Caelo	Isopropyl alcoho...	14051031	31386	40	20140214
apomix	Isopropyl alcoho...	4103112	31517	40	1505476
Hedinger	Isopropyl alcoho...	070835B	32817	40	20160712

Validation samples

A total of 156 379 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 *Isopropyl alcohol 100%*. These samples are listed above in the [calibration samples](#) section.
- 34 144 spectra from a total of 793 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Isopropyl alcohol 100%*.

Supplier	Substance	Batch	Sample ID	Spectra
zu erfassen	Isopropyl alcohol 100%	pending	30101	40
apomix	Isopropyl alcohol 100%	4103112	31517 [†]	20

- 63 534 spectra from a total of 1476 batches from further 439 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.

- 1231 spectra from 225 *Apo-Ident* customers from 584 batches from the substance/substance group *Isopropyl alcohol 100%*.

Supplier	Substance	Batch	Spectra
GEHE	Isopropyl alcohol 100%	70882B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70734B	2
Hedinger	Isopropyl alcohol 100%	70788B	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
Hedinger / Noweda	Isopropyl alcohol 100%	70703B	1
Fischar	Isopropyl alcohol 100%	1005101	1
Caelo	Isopropyl alcohol 100%	13397327	2
Gehe/Fischar	Isopropyl alcohol 100%	1005101	2
Caelo	Isopropyl alcohol 100%	14219212	3
Caelo	Isopropyl alcohol 100%	14219216	1
Caelo	Isopropyl alcohol 100%	14278904	2
Caelo	Isopropyl alcohol 100%	13336927	1
Caelo	Isopropyl alcohol 100%	1469323	1
Caelo	Isopropyl alcohol 100%	14051022	1
Caelo	Isopropyl alcohol 100%	14369313	1
Ebert & Jacobi 28.7.16	Isopropyl alcohol 100%	16137317	1
fischar	Isopropyl alcohol 100%	3346271	1
Noweda/Hedinger	Isopropyl alcohol 100%	70501B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70507B	9
Hedinger , Noweda	Isopropyl alcohol 100%	70490B	1
Otto Fischar	Isopropyl alcohol 100%	ohne	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70540B	1
Hedinger	Isopropyl alcohol 100%	705258	1
Hedinger/Noweda	Isopropyl alcohol 100%	70620B	1
Caelo	Isopropyl alcohol 100%	12031116	1
Caelo	Isopropyl alcohol 100%	70541b	2
Caelo	Isopropyl alcohol 100%	12254703	1
Caelo	Isopropyl alcohol 100%	12379504	1
Phönix	Isopropyl alcohol 100%	12321002	2
Caelo	Isopropyl alcohol 100%	12254727	2
Caelo	Isopropyl alcohol 100%	13336913	1
Caelo	Isopropyl alcohol 100%	12321030	2
Caelo	Isopropyl alcohol 100%	13148004	1
Caelo	Isopropyl alcohol 100%	12179316	1
Caelo	Isopropyl alcohol 100%		3
Caelo	Isopropyl alcohol 100%	13397305	2
Caelo	Isopropyl alcohol 100%	30011401	1
Phönix	Isopropyl alcohol 100%	15300908	1
Kassner & Sasse	Isopropyl alcohol 100%	383316	2
Hedinger	Isopropyl alcohol 100%	70562B	3
Hedinger	Isopropyl alcohol 100%	70564B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70565B	3
Hedinger/ N/ PZN:07474942	Isopropyl alcohol 100%	70598B	1
Hedinger	Isopropyl alcohol 100%	70598B	8
Hedinger	Isopropyl alcohol 100%	70593B	3
Hedinger/Phönix	Isopropyl alcohol 100%	70643B	1
Hedinger	Isopropyl alcohol 100%	70636B	2
Gutenberg-Apotheke	Isopropyl alcohol 100%	70607B	1
Hedinger Gehe	Isopropyl alcohol 100%	70673B	1
Aug. hedinger/N/PZN:074...	Isopropyl alcohol 100%	70659B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70675B	1
Hedinger/Phönix	Isopropyl alcohol 100%	706808	1
Hedinger/Anzag	Isopropyl alcohol 100%	70685B	1
Hedinger Jenne	Isopropyl alcohol 100%	706938	1
Hedinger/Gehe	Isopropyl alcohol 100%	70703B	1
Hedinger/Phoenix	Isopropyl alcohol 100%	70734B	1
Hedinger	Isopropyl alcohol 100%	70715b	1
Hedinger/Phönix	Isopropyl alcohol 100%	70715B	2
Hedinger Jenne	Isopropyl alcohol 100%	70720B	1
Hedinger/Phoenix	Isopropyl alcohol 100%	70794B	1
HedingerAlliance	Isopropyl alcohol 100%	70866B	2
Hedinger/Phoenix	Isopropyl alcohol 100%	70799B	1
HedingerAlliance	Isopropyl alcohol 100%	70881B	2
Gehe/Hedinger	Isopropyl alcohol 100%	70802B	1

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Supplier	Substance	Batch	Spectra
HedingerAlliance	Isopropyl alcohol 100%	70882B	1
Caelo	Isopropyl alcohol 100%	14219227	3
Caelo	Isopropyl alcohol 100%	14051012	3
Caelo	Isopropyl alcohol 100%	14278926	3
Caelo	Isopropyl alcohol 100%	14369302	2
Caelo	Isopropyl alcohol 100%	14369325	1
Caelo	Isopropyl alcohol 100%	14219233	1
Caelo	Isopropyl alcohol 100%	14278905	2
Caelo	Isopropyl alcohol 100%	15398828	1
Caelo	Isopropyl alcohol 100%	15171304	3
Caelo	Isopropyl alcohol 100%	16137302	2
Caelo	Isopropyl alcohol 100%	16234013	1
Caelo	Isopropyl alcohol 100%	16137317	1
Caelo	Isopropyl alcohol 100%	16137307	1
Herbasinica	Isopropyl alcohol 100%	70478b	1
Anzag	Isopropyl alcohol 100%	70471B	1
Gehe	Isopropyl alcohol 100%	70448B	1
Caelo	Isopropyl alcohol 100%	70481B	2
GEHE	Isopropyl alcohol 100%	70461B	1
Anzag	Isopropyl alcohol 100%	70459B	1
Anzag	Isopropyl alcohol 100%	70495B	1
Hedinger/ Anzag	Isopropyl alcohol 100%	70492B	1
Noweda	Isopropyl alcohol 100%	70409B	1
Otto Fischar GmbH	Isopropyl alcohol 100%	4104072	1
Jenne, Hedinger	Isopropyl alcohol 100%	70501B	1
HEDINGER/N/1.06.13/PZN...	Isopropyl alcohol 100%	70527b	1
Jenne, Hedinger	Isopropyl alcohol 100%	70519B	1
Hedinger/Gehe	Isopropyl alcohol 100%	704988	1
Hedinger/AHD	Isopropyl alcohol 100%	70527B	1
Hedinger/AHD	Isopropyl alcohol 100%	705408	1
Hedinger/Phönix	Isopropyl alcohol 100%	70520B	1
Anzag/Hedinger	Isopropyl alcohol 100%	70495B	1
SHELL	Isopropyl alcohol 100%	70540b	1
Hedinger/AHD	Isopropyl alcohol 100%	70574B	1
Hedinger Jenne	Isopropyl alcohol 100%	70545B	1
Hedinger/N/PZN:07474942	Isopropyl alcohol 100%	70559B	1
Hedinger Gehe	Isopropyl alcohol 100%	70562B	1
Hedinger/Gehe	Isopropyl alcohol 100%	7087B	1
Sanacorp	Isopropyl alcohol 100%	13050904	1
Sanacorp	Isopropyl alcohol 100%	13249410	1
Caelo	Isopropyl alcohol 100%	4031405	1
Caelo	Isopropyl alcohol 100%	4061401	1
Caelo	Isopropyl alcohol 100%	5061415	1
Caelo	Isopropyl alcohol 100%	53380	1
Caelo	Isopropyl alcohol 100%	6061402	1
Caelo	Isopropyl alcohol 100%	6061403	1
Caelo	Isopropyl alcohol 100%	6061404	1
Caelo	Isopropyl alcohol 100%	7051401	1
Hedinger / Phoenix	Isopropyl alcohol 100%	70536B	1
Hedinger , Stuttgart	Isopropyl alcohol 100%	70545B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70536B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70562B	1
Caelo	Isopropyl alcohol 100%	705538	1
Hedinger	Isopropyl alcohol 100%	70572B	5
Gehe am 07.03.14	Isopropyl alcohol 100%	70573B	1
Hedinger(Gehe)	Isopropyl alcohol 100%	70573B	1
Hedinger/Nowenda	Isopropyl alcohol 100%	70577B	2
Alliance Healthcare/Hed...	Isopropyl alcohol 100%	70578B	1
Caelo	Isopropyl alcohol 100%	70573B	1
Hedinger / Apotheke E.B...	Isopropyl alcohol 100%	70587B	1

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Supplier	Substance	Batch	Spectra
Hedinger/Gehe	Isopropyl alcohol 100%	70581B	1
Hedinger	Isopropyl alcohol 100%	70584B	3
Ichthyol/Noweda	Isopropyl alcohol 100%	70587B	1
Gehe am 17.12.2013	Isopropyl alcohol 100%	70578B	1
Hedinger/Phoenix	Isopropyl alcohol 100%	70578B	1
Hedinger	Isopropyl alcohol 100%	70592B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70587B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70593B	1
Anzag/Hedinger	Isopropyl alcohol 100%	70592B	1
Hedinger	Isopropyl alcohol 100%	70592B	1
Hedinger/ Jenne	Isopropyl alcohol 100%	70595B	1
Sanacorp	Isopropyl alcohol 100%	705988	1
Caelo	Isopropyl alcohol 100%	705988	1
Anzag/Hedinger	Isopropyl alcohol 100%	70598B	4
Caelo	Isopropyl alcohol 100%	70598B	4
GEHE 08.05.2014	Isopropyl alcohol 100%	70598B	1
Noweda / Hedinger	Isopropyl alcohol 100%	70598B	1
Isopropylalkohol GMP/Gehe	Isopropyl alcohol 100%	70598B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70598B	1
Caelo	Isopropyl alcohol 100%	70598b	1
Hedinger	Isopropyl alcohol 100%	706034	1
Hedinger	Isopropyl alcohol 100%	70603B	6
Hedinger/Sanacorp6.5.2014	Isopropyl alcohol 100%	70603B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70603B	3
Gehe/Hedinger	Isopropyl alcohol 100%	70603B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70603B	1
Hedinger/Alliance	Isopropyl alcohol 100%	70603B	3
Hedinger	Isopropyl alcohol 100%	70607B	2
Hedinger/Holdermann	Isopropyl alcohol 100%	70607B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70607B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70607B	2
Rondell Apotheke	Isopropyl alcohol 100%	70607B	2
Phoenix 22.10.14	Isopropyl alcohol 100%	70607B	1
Hedinger/ Jenne	Isopropyl alcohol 100%	70608B	1
Hedinger	Isopropyl alcohol 100%	7060B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70608B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70614B	3
Alliance/ Hedinger	Isopropyl alcohol 100%	70610B	1
HEDINGER / 20	Isopropyl alcohol 100%	70614B	1
Hedinger / Noweda	Isopropyl alcohol 100%	70620B	1
Hedinger	Isopropyl alcohol 100%	70620B	3
Hedinger/Sanacorp	Isopropyl alcohol 100%	70620B	1
A. Hedinger / Kehr	Isopropyl alcohol 100%	70614B	1
Hedinger , Stuttgart	Isopropyl alcohol 100%	70620B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70614B	1
AHD	Isopropyl alcohol 100%	70614B	1
Hedinger/ Jenne	Isopropyl alcohol 100%	70620B	1
Hedinger	Isopropyl alcohol 100%	70623B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70627B	2
Hedinger/Sanacorp	Isopropyl alcohol 100%	70627B	3
Hedinger/Anzag	Isopropyl alcohol 100%	70627B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70627B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70627B	1
Hedinger / Noweda	Isopropyl alcohol 100%	70627B	1
Hedinger	Isopropyl alcohol 100%	70627B	5
Stumpf/Hedinger	Isopropyl alcohol 100%	70627B	1
Noweda	Isopropyl alcohol 100%	70627B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70627B	1
Hedinger/Geilenkirchen	Isopropyl alcohol 100%	706388	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70638B	1

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Supplier	Substance	Batch	Spectra
Hedinger/ GEHE	Isopropyl alcohol 100%	706388	1
Hedinger/Jenne 31.10.2014	Isopropyl alcohol 100%	706388	1
Hedinger	Isopropyl alcohol 100%	70638B	3
Jenne/Hedinger	Isopropyl alcohol 100%	70643B	1
Hedinger/Noweda	Isopropyl alcohol 100%	706388	1
Hedinger	Isopropyl alcohol 100%	70643B	7
Noweda	Isopropyl alcohol 100%	70638B	1
Caelo	Isopropyl alcohol 100%	70643B	2
HEDINGER / 20	Isopropyl alcohol 100%	70638B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70638B	1
Noweda / Hedinger	Isopropyl alcohol 100%	70638B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70643B	1
AHD	Isopropyl alcohol 100%	70643B	1
Hedinger	Isopropyl alcohol 100%	70650B	5
Caelo	Isopropyl alcohol 100%	70656B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70650B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70650B	1
Hedinger	Isopropyl alcohol 100%	70656B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70656B	1
A. Hedinger / Noweda	Isopropyl alcohol 100%	70659B	2
Noweda/Hedinger	Isopropyl alcohol 100%	70659B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70659B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70659B	2
Hedinger	Isopropyl alcohol 100%	70659B	2
A.Hedinger / Kehr	Isopropyl alcohol 100%	70659B	1
Hedinger	Isopropyl alcohol 100%	70663B	2
Hedinger/Phoenix	Isopropyl alcohol 100%	70659B	2
Hedinger/Gehe	Isopropyl alcohol 100%	70663B	1
Hedinger / Noweda	Isopropyl alcohol 100%	70663B	1
Noweda/Henry Lamotte	Isopropyl alcohol 100%	70663B	1
Noweda/ Hedinger GmbH	Isopropyl alcohol 100%	70663B	1
Caelo	Isopropyl alcohol 100%	70663B	1
Hedinger	Isopropyl alcohol 100%	70666B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70668B	1
AHD /Hedinger	Isopropyl alcohol 100%	70666B	1
Hedinger	Isopropyl alcohol 100%	70668B	1
Stumpf/Hedinger	Isopropyl alcohol 100%	70673B	1
Hedinger	Isopropyl alcohol 100%	70675B	2
Hedinger / Noweda	Isopropyl alcohol 100%	70675B	1
Hedinger	Isopropyl alcohol 100%	70671B	1
Hedinger/Kehr	Isopropyl alcohol 100%	70675B	1
Caelo	Isopropyl alcohol 100%	70668B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70675B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70680B	1
Hedinger/ Noweda	Isopropyl alcohol 100%	70675B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70680B	1
Hedinger/N	Isopropyl alcohol 100%	70675B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70685	1
Caelo	Isopropyl alcohol 100%	70685B	1
Hedinger	Isopropyl alcohol 100%	70685B	6
Hedinger/Sanacorp	Isopropyl alcohol 100%	70685B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70685B	2
Phoenix goettin	Isopropyl alcohol 100%	70685B	1
Hedinger/ Noweda	Isopropyl alcohol 100%	70685B	1
Gehe	Isopropyl alcohol 100%	70685B	1
Hedinger	Isopropyl alcohol 100%	70690B	3
Hedinger	Isopropyl alcohol 100%	70693B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70693B	2
Caelo	Isopropyl alcohol 100%	70690B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70693B	1

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Supplier	Substance	Batch	Spectra
Hedinger	Isopropyl alcohol 100%	70695B	1
Caelo	Isopropyl alcohol 100%	70693B	1
August Hedinger/Phoenix	Isopropyl alcohol 100%	70695B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70696B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70696B	1
Eigen	Isopropyl alcohol 100%	70701B	1
Hedinger	Isopropyl alcohol 100%	70701B	2
Aug.Hedinger / Phoenix	Isopropyl alcohol 100%	70703B	1
Sanacorp	Isopropyl alcohol 100%	70701B	1
Hedinger/ Kehr	Isopropyl alcohol 100%	70703B	1
Hedinger	Isopropyl alcohol 100%	70703B	2
Hedinger/Anzag	Isopropyl alcohol 100%	70703B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70703B	1
Hedinger	Isopropyl alcohol 100%	70704B	1
Hedinger	Isopropyl alcohol 100%	70707B	6
Hedinger/ Gehe	Isopropyl alcohol 100%	70708B	1
Hedinger	Isopropyl alcohol 100%	70715B	4
Hedinger	Isopropyl alcohol 100%	70708B	1
A. Hedinger / Kehr	Isopropyl alcohol 100%	70715B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70720B	1
Hedinger	Isopropyl alcohol 100%	70720B	2
Audor Pharma	Isopropyl alcohol 100%	70720B	2
Hedinger/Noweda	Isopropyl alcohol 100%	70720B	1
Hedinger	Isopropyl alcohol 100%	70722B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70722B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70723B	1
Hedinger	Isopropyl alcohol 100%	70723B	1
Noweda/Hedin	Isopropyl alcohol 100%	70726B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70723B	1
HEDINGER / 20	Isopropyl alcohol 100%	70726B	1
Hedinger / Noweda	Isopropyl alcohol 100%	70734B	1
Heinger/G	Isopropyl alcohol 100%	70730B	1
Hedinger GmbH	Isopropyl alcohol 100%	70729B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70736B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70730B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70737B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70737B	2
Hedinger/Noweda	Isopropyl alcohol 100%	70737B	1
Hedinger/sanacorp	Isopropyl alcohol 100%	70739B	3
Hedinger	Isopropyl alcohol 100%	70736B	1
Hedinger	Isopropyl alcohol 100%	70737B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70736B	1
Hedinger / Sanacorp	Isopropyl alcohol 100%	70737B	1
Hedinger/AHD	Isopropyl alcohol 100%	70737B	1
Hedinger / Noweda	Isopropyl alcohol 100%	70737B	1
Hedinger/Kehr	Isopropyl alcohol 100%	7073B	1
Noweda / Hedinger	Isopropyl alcohol 100%	70742B	2
Hedinger	Isopropyl alcohol 100%	70748B	4
Hedinger	Isopropyl alcohol 100%	70742B	1
Hedinger / Noweda	Isopropyl alcohol 100%	70748B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70739B	1
Heidinger	Isopropyl alcohol 100%	70748B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70748B	1
Caelo	Isopropyl alcohol 100%	70748B	1
Noweda	Isopropyl alcohol 100%	70755B	1
Hedinger / Kehr	Isopropyl alcohol 100%	70755B	1
Hedinger/ Noweda	Isopropyl alcohol 100%	70748b	1
Caelo	Isopropyl alcohol 100%	70755B	2
Hedinger / Noweda	Isopropyl alcohol 100%	70762B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70763B	2

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Supplier	Substance	Batch	Spectra
Hedinger/Sanacorp	Isopropyl alcohol 100%	70767B	5
Hedinger	Isopropyl alcohol 100%	70767B	2
Bombastus	Isopropyl alcohol 100%	70767B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70767B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70767B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70768B	1
Hedinger / 30	Isopropyl alcohol 100%	70768B	1
Hedinger/Alliance Healt...	Isopropyl alcohol 100%	70768B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70768B	1
Aug. Hedinger GmbH & Co...	Isopropyl alcohol 100%	70768B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70771B	1
Hedinger/ Noweda	Isopropyl alcohol 100%	70771B	1
Hedinger	Isopropyl alcohol 100%	70771B	2
Hedinger	Isopropyl alcohol 100%	70783B	2
Hedinger/Sanacorp	Isopropyl alcohol 100%	70777B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70783B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70783B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70788B	2
Hedinger/AHD	Isopropyl alcohol 100%	70788B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70788B	1
Hedinger/AHD	Isopropyl alcohol 100%	70788B	1
Hedinger / Noweda	Isopropyl alcohol 100%	70788B	1
Hedinger / Alliance Hea...	Isopropyl alcohol 100%	70796B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70796B	1
Hedinger / Gehe	Isopropyl alcohol 100%	70802B	1
Hedinger	Isopropyl alcohol 100%	70809B	4
Hedinger/Gehe	Isopropyl alcohol 100%	70804B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70809B	3
Hedinger / Gehe	Isopropyl alcohol 100%	70809B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70809B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70818B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70818B	3
Hedinger/N	Isopropyl alcohol 100%	70818B	1
Hedinger/Phönix	Isopropyl alcohol 100%	70825B	1
Hedinger	Isopropyl alcohol 100%	70818B	2
Hedinger/Gehe	Isopropyl alcohol 100%	70818B	1
Rondell Apotheke	Isopropyl alcohol 100%	70818B	1
hedinger	Isopropyl alcohol 100%	70818B	1
Hedinger	Isopropyl alcohol 100%	70825B	2
Hedinger	Isopropyl alcohol 100%	70835B	1
A. Hedinger / Kehr	Isopropyl alcohol 100%	70835B	1
Hedinger/ Noweda	Isopropyl alcohol 100%	70835B	1
Hedinger / Noweda	Isopropyl alcohol 100%	70870B	1
Hedinger	Isopropyl alcohol 100%	70858B	2
Gehe	Isopropyl alcohol 100%	70835B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70853B	1
Caelo	Isopropyl alcohol 100%	70889B	1
Phönix	Isopropyl alcohol 100%	70870B	1
Fischar	Isopropyl alcohol 100%		1
Hedinger, Noweda	Isopropyl alcohol 100%	7474907	1
Caelo	Isopropyl alcohol 100%	70835B	1
Hedinger	Isopropyl alcohol 100%	70898B	1
Hedinger/ Noweda	Isopropyl alcohol 100%	70875B	1
Hedinger	Isopropyl alcohol 100%	7638B	1
Caelo	Isopropyl alcohol 100%	10061507	1
Caelo	Isopropyl alcohol 100%	10101403	1
Caelo	Isopropyl alcohol 100%	10011502	1
Spinnrad	Isopropyl alcohol 100%	1114410092	1
Caelo	Isopropyl alcohol 100%	11091401	1
Caelo	Isopropyl alcohol 100%	12041402	1

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Supplier	Substance	Batch	Spectra
Caelo	Isopropyl alcohol 100%	12081505	1
Caelo	Isopropyl alcohol 100%	13121401	1
Caelo	Isopropyl alcohol 100%	13148006	1
Caelo	Isopropyl alcohol 100%	13397314	1
Caelo	Isopropyl alcohol 100%	13336916	1
Caelo	Isopropyl alcohol 100%	13397312	2
Caelo	Isopropyl alcohol 100%	13397303	1
Caelo	Isopropyl alcohol 100%	13397317	1
Caelo	Isopropyl alcohol 100%	13397316	2
Großhandel	Isopropyl alcohol 100%	13397331	1
Caelo	Isopropyl alcohol 100%	13397330	6
Euro OTC	Isopropyl alcohol 100%	13397324	1
Caelo	Isopropyl alcohol 100%	13397318	2
Caelo	Isopropyl alcohol 100%	13397332	2
Caelo	Isopropyl alcohol 100%	13407304	1
Caelo	Isopropyl alcohol 100%	14031501	1
Caelo	Isopropyl alcohol 100%	14051008	1
Caelo	Isopropyl alcohol 100%	14051015	1
Sanacorp	Isopropyl alcohol 100%	14051017	1
Caelo	Isopropyl alcohol 100%	14051018	1
VDL	Isopropyl alcohol 100%	14051020	1
Noweda	Isopropyl alcohol 100%	14051027	1
Caelo	Isopropyl alcohol 100%	14051026	1
Sanacorp	Isopropyl alcohol 100%	14051035	1
Caelo	Isopropyl alcohol 100%	14051031	2
Caelo	Isopropyl alcohol 100%	14051034	1
Caelo	Isopropyl alcohol 100%	14051028	1
Caelo	Isopropyl alcohol 100%	140561033	1
Caelo	Isopropyl alcohol 100%	14134703	1
Bergchemie	Isopropyl alcohol 100%	14134711	1
Caelo	Isopropyl alcohol 100%	14134705	2
Caelo	Isopropyl alcohol 100%	14134720	2
Caelo	Isopropyl alcohol 100%	14134716	2
Sanacorp	Isopropyl alcohol 100%	14134709	1
Caelo	Isopropyl alcohol 100%	14134706	1
Fagron	Isopropyl alcohol 100%	14134722	1
Sanacorp	Isopropyl alcohol 100%	14134725	1
Phoenix	Isopropyl alcohol 100%	14219204	1
Caelo	Isopropyl alcohol 100%	14219202	1
Caelo	Isopropyl alcohol 100%	14219209	2
Caelo	Isopropyl alcohol 100%	14219206	1
Caelo	Isopropyl alcohol 100%	14219205	1
Caelo	Isopropyl alcohol 100%	14219211	1
Caelo	Isopropyl alcohol 100%	14219213	2
Caelo	Isopropyl alcohol 100%	14219215	2
Caelo	Isopropyl alcohol 100%	14219214	2
Caelo	Isopropyl alcohol 100%	14219218	3
Caelo	Isopropyl alcohol 100%	14219220	1
Caelo	Isopropyl alcohol 100%	14219222	1
Caelo	Isopropyl alcohol 100%	14219228	2
Caelo	Isopropyl alcohol 100%	14219224	1
Caelo	Isopropyl alcohol 100%	14278901	3
noweda	Isopropyl alcohol 100%	14278905	1
Caelo	Isopropyl alcohol 100%	14278927	1
Caelo	Isopropyl alcohol 100%	14278909	1
Caelo	Isopropyl alcohol 100%	14278929	1
Sanacorp	Isopropyl alcohol 100%	14278913	1
Caelo	Isopropyl alcohol 100%	14278907	1
Caelo	Isopropyl alcohol 100%	14278923	2
Fagron	Isopropyl alcohol 100%	14278927	1

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Supplier	Substance	Batch	Spectra
Caelo	Isopropyl alcohol 100%	14278911	2
Caelo	Isopropyl alcohol 100%	14278914	1
Sanacorp	Isopropyl alcohol 100%	14369302	3
Caelo	Isopropyl alcohol 100%	14369303	1
Caelo	Isopropyl alcohol 100%	14369306	1
Caelo	Isopropyl alcohol 100%	14369307	2
Caelo	Isopropyl alcohol 100%	14369317	1
Caelo	Isopropyl alcohol 100%	14369316	2
Caelo	Isopropyl alcohol 100%	14369322	1
Caelo	Isopropyl alcohol 100%	14369326	1
Caelo	Isopropyl alcohol 100%	14369312	1
Caelo	Isopropyl alcohol 100%	14369329	1
Caelo	Isopropyl alcohol 100%	14369334	1
Caelo	Isopropyl alcohol 100%	15057508	1
Caelo	Isopropyl alcohol 100%	15057505	1
Caelo	Isopropyl alcohol 100%	15057502	1
Caelo	Isopropyl alcohol 100%	15057507	2
Caelo	Isopropyl alcohol 100%	15057501	1
Caelo	Isopropyl alcohol 100%	15057514	1
Caelo	Isopropyl alcohol 100%	15057515	1
Caelo	Isopropyl alcohol 100%	15057511	1
Caelo	Isopropyl alcohol 100%	15057520	1
Caelo	Isopropyl alcohol 100%	15057518	1
Caelo	Isopropyl alcohol 100%	15057528	1
Caelo	Isopropyl alcohol 100%	15111401	1
Hedinger/GEHE	Isopropyl alcohol 100%	1514Q1079	1
Caelo	Isopropyl alcohol 100%	15171301	1
Caelo	Isopropyl alcohol 100%	15171303	3
Sanacorp	Isopropyl alcohol 100%	15171302	1
Caelo	Isopropyl alcohol 100%	15171305	1
Caelo	Isopropyl alcohol 100%	15171313	1
Caelo	Isopropyl alcohol 100%	15171314	1
Caelo	Isopropyl alcohol 100%	15171315	1
Caelo	Isopropyl alcohol 100%	15171327	1
Caelo	Isopropyl alcohol 100%	15171328	3
Caelo	Isopropyl alcohol 100%	15171332	1
Caelo	Isopropyl alcohol 100%	15171341	2
Caelo	Isopropyl alcohol 100%	15171340	1
Caelo	Isopropyl alcohol 100%	15171335	1
Caelo	Isopropyl alcohol 100%	15171342	2
Caelo	Isopropyl alcohol 100%	15171331	1
Caelo	Isopropyl alcohol 100%	1517308	1
Sanacorp	Isopropyl alcohol 100%	15300902	1
Caelo	Isopropyl alcohol 100%	15300904	2
Caelo	Isopropyl alcohol 100%	15300903	2
Caelo	Isopropyl alcohol 100%	15300927	2
Caelo	Isopropyl alcohol 100%	15300931	1
Caelo	Isopropyl alcohol 100%	15300918	1
Caelo	Isopropyl alcohol 100%	15300921	1
Caelo	Isopropyl alcohol 100%	15398803	1
Caelo	Isopropyl alcohol 100%	15398820	1
Caelo	Isopropyl alcohol 100%	15398814	1
Caelo	Isopropyl alcohol 100%	15398819	1
Caelo	Isopropyl alcohol 100%	15398831	2
Caelo	Isopropyl alcohol 100%	15398808	1
Caesar&Loretz/Noweda	Isopropyl alcohol 100%	15398808	1
Caelo	Isopropyl alcohol 100%	15498831	1
Caelo	Isopropyl alcohol 100%	16039901	1
Sanacorp	Isopropyl alcohol 100%	16039901	1
Caelo	Isopropyl alcohol 100%	16039902	1

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Supplier	Substance	Batch	Spectra
Caelo	Isopropyl alcohol 100%	16039904	2
Caelo	Isopropyl alcohol 100%	16039912	1
Caelo	Isopropyl alcohol 100%	16039907	1
Caelo	Isopropyl alcohol 100%	16039906	1
Caelo	Isopropyl alcohol 100%	16039913	1
Caelo	Isopropyl alcohol 100%	16039911	1
Caelo	Isopropyl alcohol 100%	16039921	1
Caelo	Isopropyl alcohol 100%	16039922	2
Caelo	Isopropyl alcohol 100%	16039925	1
Caelo	Isopropyl alcohol 100%	16039926	1
Noweda	Isopropyl alcohol 100%	16137302	1
Caelo	Isopropyl alcohol 100%	16137301	2
Caelo	Isopropyl alcohol 100%	16137303	1
Caelo	Isopropyl alcohol 100%	16137312	2
Caelo	Isopropyl alcohol 100%	16137304	1
Caelo	Isopropyl alcohol 100%	16137325	1
Caelo	Isopropyl alcohol 100%	16137336	1
Caelo	Isopropyl alcohol 100%	16234001	1
Caelo	Isopropyl alcohol 100%	16234014	1
Caelo	Isopropyl alcohol 100%	16234017	1
Caesar /phönix	Isopropyl alcohol 100%	16310603	1
Caelo	Isopropyl alcohol 100%	16234025	1
Caelo	Isopropyl alcohol 100%	163234002	1
Caelo	Isopropyl alcohol 100%	19051503	1
Caelo	Isopropyl alcohol 100%	19051405	1
Caelo	Isopropyl alcohol 100%	21111402	1
Caelo	Isopropyl alcohol 100%	25021501	1
Caelo	Isopropyl alcohol 100%	27031502	1
Caelo	Isopropyl alcohol 100%	27091401	1
Caelo	Isopropyl alcohol 100%	29011505	1
Caelo	Isopropyl alcohol 100%	29071401	1
Caelo	Isopropyl alcohol 100%	30041508	1
sophien-arzneimittel	Isopropyl alcohol 100%	310190514069	1
Caelo	Isopropyl alcohol 100%	31081501	1
Fischar/Phönix	Isopropyl alcohol 100%	4103112	1
Hedinger	Isopropyl alcohol 100%	70587B	2
Caelo	Isopropyl alcohol 100%	6324064	1
Phönix 07.01.15	Isopropyl alcohol 100%	70650B	1
hedinger	Isopropyl alcohol 100%	105208	1
Caelo	Isopropyl alcohol 100%	1071301	1
Hedinger	Isopropyl alcohol 100%	402211079	1
Caelo	Isopropyl alcohol 100%	5031303	1
Caelo	Isopropyl alcohol 100%	2011403	1
Hedinger	Isopropyl alcohol 100%	406211079	1
Caelo	Isopropyl alcohol 100%	6061320	1
Caelo	Isopropyl alcohol 100%	4091201	1
Hedinger	Isopropyl alcohol 100%	50700B	1
Caelo	Isopropyl alcohol 100%	6071201	1
Caelo	Isopropyl alcohol 100%	6081204	1
Caelo	Isopropyl alcohol 100%	6081303	1
Hedinger	Isopropyl alcohol 100%	70219B	1
Hersteller: Hedinger	Isopropyl alcohol 100%	70236B	1
Gehe	Isopropyl alcohol 100%	70382B	1
Kehr	Isopropyl alcohol 100%	70416B	1
Hedinger	Isopropyl alcohol 100%	70416B	1
Gehe	Isopropyl alcohol 100%	704098	1
Hedinger über Noweda	Isopropyl alcohol 100%	70439B	1
Hedinger/Anzag 27.02.2012	Isopropyl alcohol 100%	70417B	1
HedingerStuttgart/GEHE	Isopropyl alcohol 100%	70430B	1
Hedinger	Isopropyl alcohol 100%	70422B	1

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Supplier	Substance	Batch	Spectra
Hedinger	Isopropyl alcohol 100%	70439B	1
Caelo	Isopropyl alcohol 100%	70439B	1
Kehr	Isopropyl alcohol 100%	70439B	1
Hedinger/Holdermann 30...	Isopropyl alcohol 100%	70444B	1
Hedinger	Isopropyl alcohol 100%	70444B	1
Hedinger/ Gehe	Isopropyl alcohol 100%	70444B	1
Hedinger	Isopropyl alcohol 100%	70448B	1
Hedinger	Isopropyl alcohol 100%	70447B	2
Hedinger / Apotheke E.B. ...	Isopropyl alcohol 100%	70448B	1
Hedinger	Isopropyl alcohol 100%	70461B	3
Hedinger	Isopropyl alcohol 100%	70459B	2
Noweda	Isopropyl alcohol 100%	70459B	1
Hedinger / Apotheke E.B. ...	Isopropyl alcohol 100%	70461B	1
Hedinger	Isopropyl alcohol 100%	70457B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70457B	1
Hedinger	Isopropyl alcohol 100%	704638	1
Hedinger	Isopropyl alcohol 100%	70463B	2
Hedinger, Heiligenwiese. ...	Isopropyl alcohol 100%	70471B	1
Hedinger	Isopropyl alcohol 100%	70471B	2
Hedinger/Noweda	Isopropyl alcohol 100%	70465B	1
Hedinger	Isopropyl alcohol 100%	70465B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70471B	2
Hedinger/Anzag	Isopropyl alcohol 100%	70471B	1
Fiebig 09.11.12 EK28,33	Isopropyl alcohol 100%	704758	1
Sanacorp	Isopropyl alcohol 100%	70475B	2
Dr.Seeger GmbH	Isopropyl alcohol 100%	70475B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70475B	6
Noweda/Hedinger	Isopropyl alcohol 100%	70476B	2
Jenne, Hedinger	Isopropyl alcohol 100%	70475B	1
Klenk	Isopropyl alcohol 100%	70475b	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70476B	2
Hedinger	Isopropyl alcohol 100%	70478B	5
Hedinger/VDL	Isopropyl alcohol 100%	704788	1
Caelo	Isopropyl alcohol 100%	70478B	1
Hedinger/Gehe	Isopropyl alcohol 100%	70478B	1
Kehr	Isopropyl alcohol 100%	70478B	1
Hedinger Jenne	Isopropyl alcohol 100%	70478B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70478B	3
sanacorp	Isopropyl alcohol 100%	70481B	1
Hustadt Apotheke	Isopropyl alcohol 100%	70481B	2
Hedinger/Gehe	Isopropyl alcohol 100%	70481B	1
Hedinger /Sana	Isopropyl alcohol 100%	70488B	1
Hedinger	Isopropyl alcohol 100%	704888	1
Aug.Hedinger/Noweda	Isopropyl alcohol 100%	70488B	1
Hedinger	Isopropyl alcohol 100%	70492B	2
Hedinger/Gehe	Isopropyl alcohol 100%	70492B	1
Gehe 24.05.2013	Isopropyl alcohol 100%	70495B	1
Hedinger	Isopropyl alcohol 100%	70495B	1
Noweda	Isopropyl alcohol 100%	70490B	1
Hedinger	Isopropyl alcohol 100%	70488B	1
HedingerStuttgart/GEHE	Isopropyl alcohol 100%	704958	1
HedingerStuttgart/GEHE	Isopropyl alcohol 100%	704978	1
Hedinger	Isopropyl alcohol 100%	70497B	1
Caelo	Isopropyl alcohol 100%	70498B	3
Hedinger	Isopropyl alcohol 100%	70500B	1
Anzag 08.02.2013	Isopropyl alcohol 100%	70500B	1
Hedinger	Isopropyl alcohol 100%	70501B	4
Hedinger/Gehe	Isopropyl alcohol 100%	70501B	1
Hedinger	Isopropyl alcohol 100%	70498B	1
Hedinger/Alliance Healt. ...	Isopropyl alcohol 100%	70503B	1

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Supplier	Substance	Batch	Spectra
Hedinger/Gehe	Isopropyl alcohol 100%	70505B	1
Caesar & Loretz GmbH	Isopropyl alcohol 100%	70503B	1
Hedinger	Isopropyl alcohol 100%	70507B	7
Hedinger/Gehe	Isopropyl alcohol 100%	70507B	1
Hedinger/AHD	Isopropyl alcohol 100%	70507B	1
Gehe	Isopropyl alcohol 100%	70507B	1
Hedinger	Isopropyl alcohol 100%	70511B	3
Hedinger/ Noweda	Isopropyl alcohol 100%	70517B	1
Bombastus	Isopropyl alcohol 100%	70517B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70519B	1
Dr.Seeger GmbH	Isopropyl alcohol 100%	70519B	1
Hedinger, Heiligenwiese...	Isopropyl alcohol 100%	70519B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70519B	1
Noweda	Isopropyl alcohol 100%	70519B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70519B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70519B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70520B	1
Hedinger/ Noweda	Isopropyl alcohol 100%	70520B	1
Hedinger/Jenne	Isopropyl alcohol 100%	70525B	1
HedingerStuttgart/GEHE	Isopropyl alcohol 100%	70527B	1
Dr.Seeger GmbH	Isopropyl alcohol 100%	70527B	1
Hedinger	Isopropyl alcohol 100%	70527B	6
Stumpf/Hedinger	Isopropyl alcohol 100%	70527B	2
Anzag/Seeger	Isopropyl alcohol 100%	70527B	1
Hedinger / Noweda	Isopropyl alcohol 100%	70525B	1
Klenk	Isopropyl alcohol 100%	70527B	1
Hedinger	Isopropyl alcohol 100%	70530B	2
Alliance/ Hedinger	Isopropyl alcohol 100%	70530B	3
Hedinger	Isopropyl alcohol 100%	70532B	3
Phönix /Hedinger	Isopropyl alcohol 100%	70532B	2
Hedinger/Gehe	Isopropyl alcohol 100%	70532B	1
Hedinger/AHD	Isopropyl alcohol 100%	70532B	1
Hedinger	Isopropyl alcohol 100%	70536B	2
Caelo	Isopropyl alcohol 100%	70540B	1
Hedinger Phönix	Isopropyl alcohol 100%	70536B	1
Phönix	Isopropyl alcohol 100%	70536B	1
Caelo	Isopropyl alcohol 100%	70536B	2
Stumpf	Isopropyl alcohol 100%	70540B	1
Alliance Healthcare/Hed...	Isopropyl alcohol 100%	70536B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70540B	1
Hedinger / Apotheke E.B...	Isopropyl alcohol 100%	70541B	1
Gehe/Hedinger	Isopropyl alcohol 100%	70540B	1
Alliance/ Hedinger	Isopropyl alcohol 100%	70540B	1
Hedinger	Isopropyl alcohol 100%	70540B	1
Noweda/ Dr. Seeger	Isopropyl alcohol 100%	70540B	1
Caelo	Isopropyl alcohol 100%	70541B	2
Fagron	Isopropyl alcohol 100%	70541	1
Anzag/Hedinger	Isopropyl alcohol 100%	70541B	6
Hedinger/Sanacorp	Isopropyl alcohol 100%	70541B	1
Gehe	Isopropyl alcohol 100%	70541B	1
Hedinger	Isopropyl alcohol 100%	70541B	4
Caelo	Isopropyl alcohol 100%	70545B	1
Hedinger/ jenne	Isopropyl alcohol 100%	70541B	1
Hedinger	Isopropyl alcohol 100%	70545B	6
Hedinger/Phoenix	Isopropyl alcohol 100%	70545B	2
Hedinger/Anzag	Isopropyl alcohol 100%	70545B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70545B	1
Hedinger/Noweda	Isopropyl alcohol 100%	7054907	1
Dr.Seeger GmbH	Isopropyl alcohol 100%	70553B	2
Hedinger	Isopropyl alcohol 100%	70545b	1

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Supplier	Substance	Batch	Spectra
Hedinger	Isopropyl alcohol 100%	70553B	5
Hedinger/Gehe	Isopropyl alcohol 100%	70553B	1
Fischar	Isopropyl alcohol 100%	70553B	1
Alliance/ Hedinger	Isopropyl alcohol 100%	70553B	2
Hedinger/Anzag	Isopropyl alcohol 100%	70553B	1
Hedinger	Isopropyl alcohol 100%	705540B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70553BH	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70555B	2
Hedinger	Isopropyl alcohol 100%	70555B	4
Hedinger/ Noweda	Isopropyl alcohol 100%	70555B	1
Hedinger	Isopropyl alcohol 100%	70559B	1
Alliance/ Hedinger	Isopropyl alcohol 100%	70559B	1
Anzag/Hedinger	Isopropyl alcohol 100%	70562B	1
Caelo	Isopropyl alcohol 100%	70564B	1
Hedinger/Jenne	Isopropyl alcohol 100%	70559B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70564B	1
Hedinger , Stuttgart	Isopropyl alcohol 100%	70565B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70565B	1
Caelo	Isopropyl alcohol 100%	70565B	1
Hedinger/Anzag	Isopropyl alcohol 100%	70572B	1
Hedinger	Isopropyl alcohol 100%	70572B	2
Hedinger	Isopropyl alcohol 100%	70574B	3
Noweda/Hedinger	Isopropyl alcohol 100%	70574B	1
Alliance Healthcare/Hed...	Isopropyl alcohol 100%	70577B	1
Hedinger	Isopropyl alcohol 100%	70577B	1
Hedinger/Sanacorp	Isopropyl alcohol 100%	70578B	2
Noweda/Hedinger	Isopropyl alcohol 100%	70572B	1
Hedinger	Isopropyl alcohol 100%	70573B	1
HEDINGER / 20	Isopropyl alcohol 100%	70573B	1
Hedinger	Isopropyl alcohol 100%	70578B	2
Hedinger	Isopropyl alcohol 100%	70581B	1
Euro OTC	Isopropyl alcohol 100%	70578B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70584B	1
hedinger	Isopropyl alcohol 100%	70584B	1
Hedinger/Noweda	Isopropyl alcohol 100%	70584B	1
Hedinger/Otto	Isopropyl alcohol 100%	70581B	1
Hedinger / Noweda	Isopropyl alcohol 100%	70587B	1
Caelo	Isopropyl alcohol 100%	70593B	1
Anzag	Isopropyl alcohol 100%	7059B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70614B	1
Noweda/Hedinger	Isopropyl alcohol 100%	70610B	1
Caelo	Isopropyl alcohol 100%	713Q-01079	1
Hedinger / Sanacorp	Isopropyl alcohol 100%	707446B	1
Caelo	Isopropyl alcohol 100%	750520B	1
Caelo	Isopropyl alcohol 100%	108073	1
Caelo	Isopropyl alcohol 100%	11311602	1
Caelo	Isopropyl alcohol 100%	10121304	1
Caelo	Isopropyl alcohol 100%	9101314	1
Caelo	Isopropyl alcohol 100%	10051302	1
Caelo	Isopropyl alcohol 100%	11371204	1
Caelo	Isopropyl alcohol 100%	11371212	1
Noweda	Isopropyl alcohol 100%	11371222	1
Caelo	Isopropyl alcohol 100%	11371214	1
Hedinger	Isopropyl alcohol 100%	1207211079	1
Caelo	Isopropyl alcohol 100%	12031106	1
Caelo	Isopropyl alcohol 100%	12031129	1
Caelo	Isopropyl alcohol 100%	12112209	1
Caelo	Isopropyl alcohol 100%	11371217	1
Noweda	Isopropyl alcohol 100%	12112218	1
Gehe	Isopropyl alcohol 100%	12031105	1

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Supplier	Substance	Batch	Spectra
Noweda	Isopropyl alcohol 100%	12112213	1
Caelo	Isopropyl alcohol 100%	12091305	1
Caelo	Isopropyl alcohol 100%	12112206	1
Caelo	Isopropyl alcohol 100%	12112220	1
Caelo	Isopropyl alcohol 100%	12112224	3
Caelo	Isopropyl alcohol 100%	12179317	2
VDL	Isopropyl alcohol 100%	12179307	2
Großhandel	Isopropyl alcohol 100%	12179309	1
Caelo	Isopropyl alcohol 100%	12179311	1
Caelo	Isopropyl alcohol 100%	12179307	1
Caelo	Isopropyl alcohol 100%	12179310	1
Caelo	Isopropyl alcohol 100%	12179321	1
Caelo	Isopropyl alcohol 100%	12179328	1
Caelo	Isopropyl alcohol 100%	12179326	1
Noweda	Isopropyl alcohol 100%	12179322	1
Caelo	Isopropyl alcohol 100%	12254702	1
Caelo	Isopropyl alcohol 100%	12254708	1
Caelo	Isopropyl alcohol 100%	12254708/129	1
Caelo	Isopropyl alcohol 100%	12254709	2
Caelo	Isopropyl alcohol 100%	12254706	1
Caelo	Isopropyl alcohol 100%	12254714	1
Noweda	Isopropyl alcohol 100%	12254715	1
Gehe	Isopropyl alcohol 100%	12254718	1
Caelo	Isopropyl alcohol 100%	12254719	1
Großhandel	Isopropyl alcohol 100%	12254719	1
Noweda	Isopropyl alcohol 100%	12254724	1
Caelo	Isopropyl alcohol 100%	12254728	1
Caelo	Isopropyl alcohol 100%	12254722	1
Caelo	Isopropyl alcohol 100%	12321004	1
Caelo	Isopropyl alcohol 100%	12254724	1
Phönix 11.12.12	Isopropyl alcohol 100%	12321005	1
Caelo	Isopropyl alcohol 100%	12321008	1
Caelo	Isopropyl alcohol 100%	12321012	1
Caelo	Isopropyl alcohol 100%	12321020	2
Caelo	Isopropyl alcohol 100%	12321015	1
Caelo	Isopropyl alcohol 100%	12321016	1
Caelo	Isopropyl alcohol 100%	12321022	1
Caelo	Isopropyl alcohol 100%	12321023	3
Großhandel	Isopropyl alcohol 100%	12321026	1
Phönix/ henry lamotte	Isopropyl alcohol 100%	12321024	1
Großhandel	Isopropyl alcohol 100%	12321029	1
Anzag	Isopropyl alcohol 100%	12321028	1
Caelo	Isopropyl alcohol 100%	12379501	1
Caelo	Isopropyl alcohol 100%	12321031	1
Caelo	Isopropyl alcohol 100%	12321032	1
Caelo	Isopropyl alcohol 100%	12379502	3
Caelo	Isopropyl alcohol 100%	12379508	2
Caelo	Isopropyl alcohol 100%	12379513	1
Noweda	Isopropyl alcohol 100%	12379510	1
Caelo	Isopropyl alcohol 100%	12379515	2
Caelo	Isopropyl alcohol 100%	12379510	1
Noweda	Isopropyl alcohol 100%	12379515	1
Caelo	Isopropyl alcohol 100%	12379517	1
Caelo	Isopropyl alcohol 100%	12379518	2
Caelo	Isopropyl alcohol 100%	12379520	1
Caelo	Isopropyl alcohol 100%	12379521	2
Großhandel	Isopropyl alcohol 100%	12379525	1
Caelo	Isopropyl alcohol 100%	12379522	1
Caelo	Isopropyl alcohol 100%	12379525	2
Caelo	Isopropyl alcohol 100%	12379527	1

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Supplier	Substance	Batch	Spectra
Caelo	Isopropyl alcohol 100%	13050904	2
Phönix 15.07.2013	Isopropyl alcohol 100%	12379528	1
Caelo	Isopropyl alcohol 100%	13050901	1
Caelo	Isopropyl alcohol 100%	12379526	1
Caelo	Isopropyl alcohol 100%	13050902	1
Caelo	Isopropyl alcohol 100%	13021409	1
Caelo	Isopropyl alcohol 100%	13050907	2
Caelo	Isopropyl alcohol 100%	13050911	1
Erika apotheke	Isopropyl alcohol 100%	13050911	1
Caelo	Isopropyl alcohol 100%	13050913	1
Caelo	Isopropyl alcohol 100%	13050917	1
Caelo	Isopropyl alcohol 100%	13050916	3
Caelo	Isopropyl alcohol 100%	13050914	2
Caelo	Isopropyl alcohol 100%	13050928	1
Caelo	Isopropyl alcohol 100%	13050925	2
Caelo	Isopropyl alcohol 100%	13050922	1
Caelo	Isopropyl alcohol 100%	13071304	1
Caelo	Isopropyl alcohol 100%	13050920	1
Caelo	Isopropyl alcohol 100%	13050929	2
Caelo	Isopropyl alcohol 100%	13148012	1
Caelo	Isopropyl alcohol 100%	13148010	1
Caelo	Isopropyl alcohol 100%	13148005	1
Caelo	Isopropyl alcohol 100%	13148001	1
Caelo	Isopropyl alcohol 100%	13148015	3
Caelo	Isopropyl alcohol 100%	13148016	1
Caelo	Isopropyl alcohol 100%	13148019	3
Caelo	Isopropyl alcohol 100%	13148024	1
Großhandel	Isopropyl alcohol 100%	13148027	1
Caelo	Isopropyl alcohol 100%	13148028	1
Sanacorp	Isopropyl alcohol 100%	1324919	2
Caelo	Isopropyl alcohol 100%	13249403	2
Caelo	Isopropyl alcohol 100%	132/AKD54	1
Gehe	Isopropyl alcohol 100%	13249403	1
Caelo	Isopropyl alcohol 100%	13249405	1
Caelo	Isopropyl alcohol 100%	13249406	2
Caelo	Isopropyl alcohol 100%	13249404	1
Caelo	Isopropyl alcohol 100%	1324931	1
Caelo	Isopropyl alcohol 100%	13249407	1
Caelo	Isopropyl alcohol 100%	13249411	1
Caelo	Isopropyl alcohol 100%	13249412	2
Caelo	Isopropyl alcohol 100%	13249414	2
Caelo	Isopropyl alcohol 100%	13249413	2
Caelo	Isopropyl alcohol 100%	13249415	3
Caelo	Isopropyl alcohol 100%	13249423	1
Sanacorp	Isopropyl alcohol 100%	13249416	1
Caelo	Isopropyl alcohol 100%	13249416	1
Caelo	Isopropyl alcohol 100%	13249420	1
Caelo	Isopropyl alcohol 100%	13249430	1
Caelo	Isopropyl alcohol 100%	13249435	3
Phönix	Isopropyl alcohol 100%	13249432	1
Caelo	Isopropyl alcohol 100%	13249434	1
Caelo	Isopropyl alcohol 100%	13249437	1
Caelo	Isopropyl alcohol 100%	13249427	1
Caelo	Isopropyl alcohol 100%	13249424	1
Caelo	Isopropyl alcohol 100%	13249429	1
Caelo	Isopropyl alcohol 100%	1329421	1
Caelo	Isopropyl alcohol 100%	1329423	1
Caelo	Isopropyl alcohol 100%	13336912	2
Caelo	Isopropyl alcohol 100%	13336911	1
Caelo	Isopropyl alcohol 100%	13336922	1

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Supplier	Substance	Batch	Spectra
Caelo	Isopropyl alcohol 100%	13336924	1
Caelo	Isopropyl alcohol 100%	13336934	1
Großhandel	Isopropyl alcohol 100%	13336935	2
Caelo	Isopropyl alcohol 100%	13336938	3
Caelo	Isopropyl alcohol 100%	13336930	1
Caelo	Isopropyl alcohol 100%	13336936	1
cealo	Isopropyl alcohol 100%	13336936	1
Caelo	Isopropyl alcohol 100%	13336933	1
Caelo	Isopropyl alcohol 100%	13336939	2
Caelo	Isopropyl alcohol 100%	13336941	2
Caelo	Isopropyl alcohol 100%	13336944	1
Caelo	Isopropyl alcohol 100%	13336942	1
Caelo	Isopropyl alcohol 100%	13336943	2
Caelo	Isopropyl alcohol 100%	13336945	1
Noweda	Isopropyl alcohol 100%	13397303	1
Caelo	Isopropyl alcohol 100%	13397311	1
Caelo	Isopropyl alcohol 100%	13397304	2
Caelo	Isopropyl alcohol 100%	13397323	1
Phonix	Isopropyl alcohol 100%	14134715	1
Fagron	Isopropyl alcohol 100%	14134702	1
Anzag	Isopropyl alcohol 100%	14219233	1
Caelo	Isopropyl alcohol 100%	14369370	1
Hedinger	Isopropyl alcohol 100%	1512211079	1
Caelo	Isopropyl alcohol 100%	15398806	1
Caelo	Isopropyl alcohol 100%	15398813	1
Caelo	Isopropyl alcohol 100%	16011406	1
Hedinger	Isopropyl alcohol 100%	1601311079	1
Celo	Isopropyl alcohol 100%	16039937	1
Celo	Isopropyl alcohol 100%	16039925	1
Caelo	Isopropyl alcohol 100%	16137308	1
Caelo	Isopropyl alcohol 100%	21021311	1
Caelo	Isopropyl alcohol 100%	18041306	1
Caelo	Isopropyl alcohol 100%	22011302	1
Caelo	Isopropyl alcohol 100%	2201201301	1
Hedinger	Isopropyl alcohol 100%	2x070461B	1
Caelo	Isopropyl alcohol 100%	22121201	1
Caelo	Isopropyl alcohol 100%	20081204	1
Caelo	Isopropyl alcohol 100%	20060912-4	1
Caelo	Isopropyl alcohol 100%	22111204	1
Caelo	Isopropyl alcohol 100%	22091203	1
Hedinger	Isopropyl alcohol 100%	2310211079	1
Caelo	Isopropyl alcohol 100%	25061201	1
Caelo	Isopropyl alcohol 100%	24071201	1
Caelo	Isopropyl alcohol 100%	29101304	1
Hedinger	Isopropyl alcohol 100%	3013E1079	1
Caelo	Isopropyl alcohol 100%	28081302	1
Caelo	Isopropyl alcohol 100%	30111303	1
Caelo	Isopropyl alcohol 100%	29051202	1
Caelo	Isopropyl alcohol 100%	28021316	1
kost	Isopropyl alcohol 100%	310120913059	2
Kost/ - /16.09.13	Isopropyl alcohol 100%	310120913059	1
Kost/kost/sophien	Isopropyl alcohol 100%	310261113062	1
Caelo	Isopropyl alcohol 100%	31101204	1
Fischer/Phönix	Isopropyl alcohol 100%	4103014	1
Aug. Hedinger GmbH & Co...	Isopropyl alcohol 100%	501114B	1
Gehe 12.04.2013	Isopropyl alcohol 100%	4912Q-07001	1
Caelo	Isopropyl alcohol 100%	543892	1
spinnenrad	Isopropyl alcohol 100%	611410093	1
Caelo	Isopropyl alcohol 100%	7272262	1
hedinger/anzag	Isopropyl alcohol 100%	705838	1

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Supplier	Substance	Batch	Spectra
Hedinger/Otto	Isopropyl alcohol 100%		1
Hedinger	Isopropyl alcohol 100%	7474942	1
Caelo	Isopropyl alcohol 100%	7411	1
Fagron	Isopropyl alcohol 100%		1
Caelo	Isopropyl alcohol 100%	7776	1

- 57 210 spectra from 332 *Apo-Ident* customers from a total of 19 515 batches from a further 328 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 *Isopropyl alcohol 100%* 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 *Isopropyl alcohol 100%* 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	34 144
Type B	0	60	0	63 534
Type C	0	1189	42	57 210

The substance/substance group *Isopropyl alcohol 100%* 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 % (> 99.9690 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.5963 %)	96.5881 % (> 96.3444 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30759	31517	5.92	213.94
31232	31517	1.46	210.84
31386	31517	3.00	212.76
31517	31517	0.00	210.10
32817	31517	6.09	202.27

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Isopropyl alcohol 70%**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30848-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Isopropyl alcohol 70%; Alcohol isopropylicus 70%

Special notes

When selecting the *Isopropyl alcohol 70%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Isopropyl alcohol 70%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Isopropyl alcoho...	14076503	31388	40	1412279
Caelo	Isopropyl alcoho...	14331004	31622	40	20141104
Caelo	Isopropyl alcoho...	15403802	31831	40	20151127
Caelo	Isopropyl alcoho...	163189	33105	40	20161206*

Validation samples

A total of 156379 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 *Isopropyl alcohol 70%*. These samples are listed above in the [calibration samples](#) section.
- 34184 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 440 spectra of 12 reference samples from the substance/substance group *Isopropyl alcohol 70%*.

Supplier	Substance	Batch	Sample ID	Spectra
zu erfassen	Isopropyl alcohol 70%	pending	30391	40
Hofmann's	Isopropyl alcohol 70%	301012	30848	40
Caelo	Isopropyl alcohol 70%	14331004	31622 [†]	20
Caelo	Isopropyl alcohol 70%	15403802	31831 [†]	20
Caelo	Isopropyl alcohol 70%	160884	32216	40
Caelo	Isopropyl alcohol 70%	161678	32318	40
Caelo	Isopropyl alcohol 70%	161677	32319	40
Caelo	Isopropyl alcohol 70%	161676	32320	40
Caelo	Isopropyl alcohol 70%	161679	32322	40
Caelo	Isopropyl alcohol 70%	163190	33106	40
Caelo	Isopropyl alcohol 70%	163191	33107	40
Caelo	Isopropyl alcohol 70%	163192	33108	40

- 63154 spectra from a total of 1466 batches from further 439 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](#).

*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.

[†]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*.

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.

- 813 spectra from 113 *Apo-Ident* customers from 623 batches from the substance/substance group *Isopropyl alcohol 70%*.

Supplier	Substance	Batch	Spectra
A. Hedinger/Noweda	Isopropyl alcohol 70%	53336	2
Caelo	Isopropyl alcohol 70%	13363101	2
Eigenherstellung Hubert...	Isopropyl alcohol 70%	2014072221 (DF)	1
Caelo	Isopropyl alcohol 70%	2415Q-01080	1
Hustadt-Apotheke	Isopropyl alcohol 70%	160413/2	1
Fischar	Isopropyl alcohol 70%	4114064	1
Rondell Apotheke	Isopropyl alcohol 70%	3215M-07123	1
Fischar	Isopropyl alcohol 70%	2183	1
Caelo	Isopropyl alcohol 70%	2314E-01080	1
Wolf-Apotheke / Defektur	Isopropyl alcohol 70%	41017/50W1o	1
Caelo	Isopropyl alcohol 70%	3414E-01080	1
Fischar / Anzag	Isopropyl alcohol 70%	4115073	1
Otto Fischar GmbH & Co...	Isopropyl alcohol 70%	4115114	2
Caelo	Isopropyl alcohol 70%	4914A-01080	1
Eigen	Isopropyl alcohol 70%	5216E-01079	1
Rondell Apotheke	Isopropyl alcohol 70%	4814E-07123	1
Martinus-Apotheke	Isopropyl alcohol 70%	A-021116-2D	1
Caelo	Isopropyl alcohol 70%	Caelo	1
Fagron	Isopropyl alcohol 70%	4114104	1
Hedinger/Anzag	Isopropyl alcohol 70%	303008	1
Winthrop	Isopropyl alcohol 70%	2600750T	1
Fischar/Sanacorp	Isopropyl alcohol 70%	4114044	1
Labor	Isopropyl alcohol 70%	7939	1
Wintrop AM GmbH	Isopropyl alcohol 70%	2600749T	1
Eigenherstellung	Isopropyl alcohol 70%	9091115	1
Eigenherstellung	Isopropyl alcohol 70%	9261114	1
Eigenherstellung	Isopropyl alcohol 70%	9211215	1
Eigenherstellung	Isopropyl alcohol 70%	9270215	1
Hedinger/AHD	Isopropyl alcohol 70%	53326	1
Eigenherstellung	Isopropyl alcohol 70%	9100414	1
Gutenberg-Apotheke	Isopropyl alcohol 70%	140612014	1
Caelo	Isopropyl alcohol 70%	14229202	1
Caelo	Isopropyl alcohol 70%	15192003	2
Caelo	Isopropyl alcohol 70%	15308201	1
Caelo	Isopropyl alcohol 70%	15150202	3
Caelo	Isopropyl alcohol 70%	15404002	2
Caelo	Isopropyl alcohol 70%	1915A-01080	1
Caelo	Isopropyl alcohol 70%	RH141030-0003	1
Eigenherstellung	Isopropyl alcohol 70%	9070313	1
Eigenherstellung	Isopropyl alcohol 70%	9010813	1
Eigenherstellung	Isopropyl alcohol 70%	9230413	1
Hedinger	Isopropyl alcohol 70%	HA32	1
Fischar	Isopropyl alcohol 70%	4114082	1
GEHE	Isopropyl alcohol 70%	221160/3	1
Gehe	Isopropyl alcohol 70%	11370004	3
GEHE	Isopropyl alcohol 70%	12037601	1
GEHE	Isopropyl alcohol 70%	12136303	5
Eigenproduktion	Isopropyl alcohol 70%	2413E-01080	1
Brugger	Isopropyl alcohol 70%	21112013	1
Defektur	Isopropyl alcohol 70%	21012013	1
Eigenherstellung	Isopropyl alcohol 70%	3313Q-01080	1
GEHE	Isopropyl alcohol 70%	603117000	1

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Supplier	Substance	Batch	Spectra
Eigenherstellung	Isopropyl alcohol 70%	1513A-01080	1
Wolf-Apotheke	Isopropyl alcohol 70%		4
N.N.	Isopropyl alcohol 70%		1
eigene Herstellung	Isopropyl alcohol 70%	91215	1
Eigenherstellung	Isopropyl alcohol 70%	1-23102014	1
Caelo	Isopropyl alcohol 70%	116M-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	216A-01080	1
Defektur	Isopropyl alcohol 70%	2/15	1
Eigenherstellung	Isopropyl alcohol 70%	1-20082014	1
Apotheke	Isopropyl alcohol 70%	116E-07013	1
Eigenherstellung	Isopropyl alcohol 70%	1-11122014	1
Eigenherstellung	Isopropyl alcohol 70%	316E	1
Eigenherstellung	Isopropyl alcohol 70%	216M-01080	1
Caelo	Isopropyl alcohol 70%	2041501	1
Eigen Defektur	Isopropyl alcohol 70%	316Q-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	216M-01080	1
Caelo	Isopropyl alcohol 70%	3081605	1
Caelo	Isopropyl alcohol 70%	5061501	1
Rondell Apotheke	Isopropyl alcohol 70%	245Q-07123	1
Eigenherstellung	Isopropyl alcohol 70%	4022016-01	1
Hirsch Apotheke	Isopropyl alcohol 70%	415M-0108	1
Defekur	Isopropyl alcohol 70%	516Q-01080	1
Hedinger/GEHE	Isopropyl alcohol 70%	53266	1
Gehe	Isopropyl alcohol 70%	53264	1
Eigenherstellung	Isopropyl alcohol 70%	517Q-01080	1
Eigenherstellung	Isopropyl alcohol 70%	515E-01080	1
Phoenix 17.03.2014	Isopropyl alcohol 70%	53280	1
gehe	Isopropyl alcohol 70%	53270	1
Hedinger/AHD	Isopropyl alcohol 70%	53277	1
Alliance Health 17.03.2...	Isopropyl alcohol 70%	53279	2
Anzag/Hedinger	Isopropyl alcohol 70%	53285	3
GEHE am 17.06.2014	Isopropyl alcohol 70%	53286	1
Gehe	Isopropyl alcohol 70%	53290	1
Herding/AHD	Isopropyl alcohol 70%	53296	1
Gehe	Isopropyl alcohol 70%	53296	1
GEHE am 16.08.2014	Isopropyl alcohol 70%	53297	1
Hedinger / Noweda	Isopropyl alcohol 70%	53300	1
Hedinger	Isopropyl alcohol 70%	53303	1
Gehe	Isopropyl alcohol 70%	53303	1
Phönix 05.01.15	Isopropyl alcohol 70%	53303	1
AHD/Hedinger	Isopropyl alcohol 70%	53296	1
Hedinger	Isopropyl alcohol 70%	53308	1
Hedinger	Isopropyl alcohol 70%	53306	1
Hedinger / Noweda	Isopropyl alcohol 70%	5331	1
Hedinger/AHD	Isopropyl alcohol 70%	53310	1
Hedinger/Noweda	Isopropyl alcohol 70%	53310	1
AHD/Hedinger	Isopropyl alcohol 70%	53318	1
Gehe/Hedinger	Isopropyl alcohol 70%	53310	1
Hedinger	Isopropyl alcohol 70%	53316	1
Hedinger GmbH & Co. KG/...	Isopropyl alcohol 70%	53328	1
Hedinger / Noweda	Isopropyl alcohol 70%	53324	1
Hedinger / Noweda	Isopropyl alcohol 70%	53321	1
Hedinger/AHD	Isopropyl alcohol 70%	53322	1
Phoenix/AHD	Isopropyl alcohol 70%	53329	1
Hedinger/Phoenix	Isopropyl alcohol 70%	53332	1
Hedinger GmbH & Co. KG/...	Isopropyl alcohol 70%	53329	1
Caelo	Isopropyl alcohol 70%	53332	1
Hedinger / Gehe	Isopropyl alcohol 70%	53337	1
Hedinger/AHD	Isopropyl alcohol 70%	53340	1
Hedinger	Isopropyl alcohol 70%	53340	1

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Supplier	Substance	Batch	Spectra
HEDINGER / Noweda	Isopropyl alcohol 70%	53340	1
Phönix/Hedinger	Isopropyl alcohol 70%	53341	1
Hedinger/AHD	Isopropyl alcohol 70%	53346	1
Gehe/Hedinger26.04.16	Isopropyl alcohol 70%	53359	1
Hedinger/Noweda	Isopropyl alcohol 70%	53360	1
Noweda/Hedinger	Isopropyl alcohol 70%	53350	1
Gehe/Hedinger29.08.2016	Isopropyl alcohol 70%	53372	1
Hedinger/Phoenix	Isopropyl alcohol 70%	53367	1
Hedinger/AHD	Isopropyl alcohol 70%	53355	1
Hedinger	Isopropyl alcohol 70%	53363	1
Hedinger/ Kehr	Isopropyl alcohol 70%	53377	1
Hedinger/Phoenix	Isopropyl alcohol 70%	53377	1
Hedinger/Phoenix	Isopropyl alcohol 70%	53382	1
Caelo	Isopropyl alcohol 70%	53383	2
Hedinger/Noweda	Isopropyl alcohol 70%	53380	1
Hedinger/Kehr	Isopropyl alcohol 70%	53393	1
Hedinger/Gehe	Isopropyl alcohol 70%	53385	1
Caelo	Isopropyl alcohol 70%	53385	1
Hedinger/Kehr	Isopropyl alcohol 70%	53386	1
Hedinger / Noweda	Isopropyl alcohol 70%	53385	1
Caelo	Isopropyl alcohol 70%	53398	1
Eiegn/Defektur	Isopropyl alcohol 70%	616E-01080	1
Caelo	Isopropyl alcohol 70%	53408	1
Caelo	Isopropyl alcohol 70%	6061401	1
Hedinger/Noweda	Isopropyl alcohol 70%	53395	1
Caelo	Isopropyl alcohol 70%	6081405	1
Herstellung in Apotheke	Isopropyl alcohol 70%	70587B	1
Rondell Apotheke	Isopropyl alcohol 70%	716M-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	716M-01080	1
Gehe/Hedinger	Isopropyl alcohol 70%	83366	1
Labor	Isopropyl alcohol 70%		4
HirschApotheke	Isopropyl alcohol 70%	10151-01080	1
Caelo	Isopropyl alcohol 70%	11031406	1
Rondell	Isopropyl alcohol 70%	1014M-07123	1
Eigen Defektur	Isopropyl alcohol 70%	1016E-01080	1
Caelo	Isopropyl alcohol 70%	1016A	1
Caelo	Isopropyl alcohol 70%	11051501	1
Eigen/Defektur	Isopropyl alcohol 70%	1116M-01080	1
Caelo	Isopropyl alcohol 70%	113363003	1
Hergestellt	Isopropyl alcohol 70%	1150727	1
Caelo	Isopropyl alcohol 70%	12031514	1
Defektur	Isopropyl alcohol 70%	12/15	1
Caelo	Isopropyl alcohol 70%	1160113	1
Caelo	Isopropyl alcohol 70%	12031515	1
Rezeptur	Isopropyl alcohol 70%	1150617	1
Apotheke	Isopropyl alcohol 70%	12345	1
Rondell Apotheke	Isopropyl alcohol 70%	1115Q-07123	1
Defektur	Isopropyl alcohol 70%	1214I	1
Defektur	Isopropyl alcohol 70%	1215A	1
Wolf-Apotheke / Defektur	Isopropyl alcohol 70%	123456	2
Caelo	Isopropyl alcohol 70%	123456789	1
Rondell Apotheke	Isopropyl alcohol 70%	1316I-01080	1
Rondell Apotheke	Isopropyl alcohol 70%	1316I-01080	2
Caelo	Isopropyl alcohol 70%	13319404	2
Caelo	Isopropyl alcohol 70%	13363107	1
Caelo	Isopropyl alcohol 70%	140226402	1
Caelo	Isopropyl alcohol 70%	14026401	4
Defektur	Isopropyl alcohol 70%	14/14	1
Gehe/Phönix	Isopropyl alcohol 70%	136363003	1
Caelo	Isopropyl alcohol 70%	14026402	5

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Supplier	Substance	Batch	Spectra
Caelo	Isopropyl alcohol 70%	14026403	2
Stern-Defektur	Isopropyl alcohol 70%	140310001	1
Hetterich	Isopropyl alcohol 70%	140403	1
Stern-Defektur	Isopropyl alcohol 70%	140404005	1
Caelo	Isopropyl alcohol 70%	140505	1
Caelo	Isopropyl alcohol 70%	14041501	1
STERN	Isopropyl alcohol 70%	140507002	1
Caelo	Isopropyl alcohol 70%	14074205	1
Caelo	Isopropyl alcohol 70%	14076602	6
STERN	Isopropyl alcohol 70%	140617002	1
Caelo	Isopropyl alcohol 70%	14076501	1
Caelo	Isopropyl alcohol 70%	14076603	2
Caelo	Isopropyl alcohol 70%	14101402	1
Caelo	Isopropyl alcohol 70%	14114501	1
Caelo	Isopropyl alcohol 70%	14114601	2
Hustadt Apotheke	Isopropyl alcohol 70%	141211	1
Leyh Pharma	Isopropyl alcohol 70%	141311	1
Caelo	Isopropyl alcohol 70%	14146701	3
Caelo	Isopropyl alcohol 70%	14146801	3
Caelo	Isopropyl alcohol 70%	14146703	1
Caelo	Isopropyl alcohol 70%	14146802	1
Caelo	Isopropyl alcohol 70%	14146803	6
Defektur	Isopropyl alcohol 70%	1415M-01080	1
Defektur	Isopropyl alcohol 70%	1414I	1
Caelo	Isopropyl alcohol 70%	1416702	1
Eigenherstellung	Isopropyl alcohol 70%	1416E-01080	1
Defektur/eigen	Isopropyl alcohol 70%	1416Q-01080	1
Caelo	Isopropyl alcohol 70%	14229101	4
Caelo	Isopropyl alcohol 70%	14229103	2
Sanacorp	Isopropyl alcohol 70%	14267805	1
Caelo	Isopropyl alcohol 70%	14327203	1
Caelo	Isopropyl alcohol 70%	14330802	1
Caelo	Isopropyl alcohol 70%	14330803	2
Caelo	Isopropyl alcohol 70%	14331003	3
Caelo	Isopropyl alcohol 70%	14330901	1
Caelo	Isopropyl alcohol 70%	14330902	1
Caelo	Isopropyl alcohol 70%	14331004	2
Leyh Pharma	Isopropyl alcohol 70%	143541	1
Caelo	Isopropyl alcohol 70%	15014102	3
Caelo	Isopropyl alcohol 70%	15014101	1
Caelo	Isopropyl alcohol 70%	15014202	2
Caelo	Isopropyl alcohol 70%	15014204	1
Caelo	Isopropyl alcohol 70%	15053505	1
Caelo	Isopropyl alcohol 70%	15014301	1
Caelo	Isopropyl alcohol 70%	15014302	2
EuroPTC/Phönix	Isopropyl alcohol 70%	15076401	2
Caelo	Isopropyl alcohol 70%	15076401	2
Fagron	Isopropyl alcohol 70%	15076501	1
Caelo	Isopropyl alcohol 70%	15076601	1
Caelo	Isopropyl alcohol 70%	15076602	7
Caelo	Isopropyl alcohol 70%	15076603	2
Hustadt-Apotheke	Isopropyl alcohol 70%	151204	1
Schwanen-Apothek-Köster	Isopropyl alcohol 70%	151028-1	1
Caelo	Isopropyl alcohol 70%	15150201	1
Defektur	Isopropyl alcohol 70%	1516M-01080	1
Caelo	Isopropyl alcohol 70%	15192001	2
Caelo	Isopropyl alcohol 70%	15191902	2
Caelo	Isopropyl alcohol 70%	15192002	2
Caelo	Isopropyl alcohol 70%	15192101	2
Leyh Pharms	Isopropyl alcohol 70%	152521	1

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Supplier	Substance	Batch	Spectra
Caelo	Isopropyl alcohol 70%	15192102	1
Leyh Pharma	Isopropyl alcohol 70%	152121	1
Caelo	Isopropyl alcohol 70%	15309001	4
Caelo	Isopropyl alcohol 70%	15309101	1
Caelo	Isopropyl alcohol 70%	15403802	5
Caelo	Isopropyl alcohol 70%	15437801	1
Leyh Pharma	Isopropyl alcohol 70%	154531	1
Caelo	Isopropyl alcohol 70%	15403902	1
Caelo	Isopropyl alcohol 70%	15437601	2
Schwanen-Apotheke, Köster	Isopropyl alcohol 70%	160104-1	1
Leyh Pharma	Isopropyl alcohol 70%	155021	1
Caelo	Isopropyl alcohol 70%	16071503	1
Caelo	Isopropyl alcohol 70%	16052014-100	1
Caelo	Isopropyl alcohol 70%	16121402	1
Caelo	Isopropyl alcohol 70%	16088302	1
Caelo	Isopropyl alcohol 70%	16121403	1
Hirsch Apotheke	Isopropyl alcohol 70%	1615I-01080	1
Ichthyol über Phoenix	Isopropyl alcohol 70%	16167802	1
Defektur 1616E-01080	Isopropyl alcohol 70%	1616E-01080	1
Kastner	Isopropyl alcohol 70%	1714I-01080	1
Sonnen-Apotheke Wefensl...	Isopropyl alcohol 70%	17/2015	1
Caelo	Isopropyl alcohol 70%	18031503	1
Defektur	Isopropyl alcohol 70%	1716A-01080	1
Caelo	Isopropyl alcohol 70%	18061509	1
Caelo	Isopropyl alcohol 70%	18081510	1
Caelo	Isopropyl alcohol 70%	18031504	1
Caelo	Isopropyl alcohol 70%	18061508	1
Caelo	Isopropyl alcohol 70%	18081511	1
Eigenherstellung	Isopropyl alcohol 70%		3
Eigenherstellung	Isopropyl alcohol 70%	1815E-01080	1
Caelo	Isopropyl alcohol 70%	19111401	1
HirschApotheke	Isopropyl alcohol 70%	1815E-01080	1
Caelo	Isopropyl alcohol 70%	19111402	1
Eigen/Defektur	Isopropyl alcohol 70%	1916M-01080	1
Eigenherstellung	Isopropyl alcohol 70%	1916A	1
Eigenherstellung	Isopropyl alcohol 70%	1953	1
Caelo	Isopropyl alcohol 70%	20011503	1
Caelo	Isopropyl alcohol 70%	20021506	1
Ottlik	Isopropyl alcohol 70%	2015090420	1
Eigenherstellung	Isopropyl alcohol 70%	2015E-01080	1
Defektur/eigen	Isopropyl alcohol 70%	2216A-01080	1
Defektur	Isopropyl alcohol 70%	2216B-01080	1
Caelo	Isopropyl alcohol 70%	21114103	1
Eigenherstellung	Isopropyl alcohol 70%	2016040520KS	1
Eigenherstellung	Isopropyl alcohol 70%	23/15	2
Caelo	Isopropyl alcohol 70%	2015181201EO	1
Eigenherstellung	Isopropyl alcohol 70%	2216E-01080	1
Defektur	Isopropyl alcohol 70%	22/14	1
HirschApotheke	Isopropyl alcohol 70%	2315I-01080	1
Winthorp AM/NOW	Isopropyl alcohol 70%	2600790T	1
Caelo	Isopropyl alcohol 70%	23061501	1
Eigen	Isopropyl alcohol 70%	2416M-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	2316I-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	2516I-01080	1
Caelo	Isopropyl alcohol 70%	23061502	1
Caelo	Isopropyl alcohol 70%	25091402	1
Caelo	Isopropyl alcohol 70%	25081401	1
Isopropylalkohol GMP/Gehe	Isopropyl alcohol 70%	2314M-01080	1
Winthrop Arzneimittel G...	Isopropyl alcohol 70%	2600802T	1
Winthrop/Alliance Healt...	Isopropyl alcohol 70%	2600875T	1

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Supplier	Substance	Batch	Spectra
Winthrop Arzneimittel G...	Isopropyl alcohol 70%	2600857T	1
Zentiva/Alliance Health...	Isopropyl alcohol 70%	2600866T	1
Winthrop/Alliance Healt...	Isopropyl alcohol 70%	2600892t	1
Zentiva/Alliance Health...	Isopropyl alcohol 70%	2600887T	1
Winthrop	Isopropyl alcohol 70%	2600846T	1
Zentiva/Alliance Health...	Isopropyl alcohol 70%	2600906T	2
Winthrop Arzneimittel G...	Isopropyl alcohol 70%	2600916T	1
Winthrop	Isopropyl alcohol 70%	2600938T	1
Rondell Apotheke	Isopropyl alcohol 70%	2615E-07123	1
Zentiva/Alliance Health...	Isopropyl alcohol 70%	2600948T	1
Winthrop	Isopropyl alcohol 70%	2600977T	1
Zentiva/Alliance Health...	Isopropyl alcohol 70%	2600953T	1
Caelo	Isopropyl alcohol 70%	2616E-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	2616Q-01080	1
Winthrop Arzneimittel G...	Isopropyl alcohol 70%	2600915T	1
Caelo	Isopropyl alcohol 70%	26071401	1
Eigen/Defektur	Isopropyl alcohol 70%	2716A-01080	1
Caelo	Isopropyl alcohol 70%	2716I-01080	1
Defektur	Isopropyl alcohol 70%	28/14	1
Eigenherstellung	Isopropyl alcohol 70%	28072014	1
Rondell Apotheke	Isopropyl alcohol 70%	2814E-07123	1
Defektur/eigen	Isopropyl alcohol 70%	2816M-01080	1
Apotheke	Isopropyl alcohol 70%	2815E-01080	1
M.Kastner	Isopropyl alcohol 70%	2914M-01080	1
Defektur	Isopropyl alcohol 70%	2915E	1
Rondell Apotheke	Isopropyl alcohol 70%	3016E-01080	1
Defektur/eigen	Isopropyl alcohol 70%	3016E-01080	1
Eigenherstellung	Isopropyl alcohol 70%	3116I-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	3016M-01080	1
eigenherstellung	Isopropyl alcohol 70%	3116Q-03043	1
Eigenherstellung	Isopropyl alcohol 70%	3215E-01080	1
Caelo	Isopropyl alcohol 70%	3216E	2
Caelo	Isopropyl alcohol 70%	3115E-01080	1
Defektur/eigen	Isopropyl alcohol 70%	3216I-01080	1
Sonnen-Apotheke Wefensl...	Isopropyl alcohol 70%	33/15	1
Eigenherstellung	Isopropyl alcohol 70%	3414E-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	3515A-01080	1
Apotheke	Isopropyl alcohol 70%	3366	1
wir leben Apotheke Tespe	Isopropyl alcohol 70%	3415M-01080	1
Defektur	Isopropyl alcohol 70%	34/14	1
M.Kastner	Isopropyl alcohol 70%	3314I-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	3516M-01080	1
Eigen	Isopropyl alcohol 70%	3615A-01080	1
eigen	Isopropyl alcohol 70%	3615I-01080	1
Eigen	Isopropyl alcohol 70%	3616M-01080	1
Frau Morgulis	Isopropyl alcohol 70%	3614E-01080	1
Defektur	Isopropyl alcohol 70%	3715Q	1
Rondell-Apotheke	Isopropyl alcohol 70%	3814Q-07123	1
Defektur	Isopropyl alcohol 70%	37/14	1
Rondell Apotheke	Isopropyl alcohol 70%	3816A-01080	1
Labor	Isopropyl alcohol 70%	3866	1
Eigen	Isopropyl alcohol 70%	3914A-01080	1
Wolf-Apotheke / Defektur	Isopropyl alcohol 70%	41125/1Hk	1
Eigene	Isopropyl alcohol 70%	3815A-01080	1
Defektur/Wolf-Apotheke	Isopropyl alcohol 70%	40509/50Wo	1
Wolf-Apotheke / Defektur	Isopropyl alcohol 70%	40729/50Hk	1
Kastner (eigen)	Isopropyl alcohol 70%	3914A-01080	1
Fischar	Isopropyl alcohol 70%	4114041	1
Defektur	Isopropyl alcohol 70%	4114I	1
Eigenherstellung	Isopropyl alcohol 70%	4115A-01080	1

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Supplier	Substance	Batch	Spectra
Eigenherstellung	Isopropyl alcohol 70%	4114Q-01080	1
Otto Fischar GmbH & Co....	Isopropyl alcohol 70%	4115012	1
Defektur	Isopropyl alcohol 70%	4115Q	1
Wolf-Apotheke / Defektur	Isopropyl alcohol 70%	41212/50Si	1
Eigen	Isopropyl alcohol 70%	4215E-01080	1
Rondell Apotheke	Isopropyl alcohol 70%	4215E-07123	1
Eigen/Defektur	Isopropyl alcohol 70%	4215M-01080	1
Defektur	Isopropyl alcohol 70%	43/14	1
Defektur	Isopropyl alcohol 70%	4315Q-01080	1
Defektur	Isopropyl alcohol 70%	4415A-01080	1
Defektur 4416A-01080	Isopropyl alcohol 70%	4416A-01080	1
HirschApotheke	Isopropyl alcohol 70%	4514I-01080	1
Hirsch Apotheke	Isopropyl alcohol 70%	4714I-01080	1
Eigenherstellung	Isopropyl alcohol 70%	4515Q-01080	1
Defektur	Isopropyl alcohol 70%	4714M	1
Eigenherstellung	Isopropyl alcohol 70%	4715M	1
Eigen/Defektur	Isopropyl alcohol 70%	4715E-01080	1
Defektur 4814N-01080	Isopropyl alcohol 70%	4814N-01080	2
Eigenherstellung	Isopropyl alcohol 70%	4716Q-01080	1
Eigenherstellung	Isopropyl alcohol 70%	5015Q-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	5015A-01080	1
Defektur/Wolf-Apotheke	Isopropyl alcohol 70%	50103/50Wlo	1
Rondell Apotheke	Isopropyl alcohol 70%	4815M-01080	1
Apotärze	Isopropyl alcohol 70%	4815I-01080	1
Eigen/Defektur	Isopropyl alcohol 70%	4815Q-01080	1
Wolf-Apotheke / Defektur	Isopropyl alcohol 70%	50204/50Bz	1
Defektur/Wolf-Apotheke	Isopropyl alcohol 70%	50227/50Wlo	1
Defektur/Wolf-Apotheke	Isopropyl alcohol 70%	50330/50Wlo	1
Defektur/Wolf-Apotheke	Isopropyl alcohol 70%	50715/50Wlo	1
CL. LANGE	Isopropyl alcohol 70%	50921/51LA	1
Defektur/Wolf-Apotheke	Isopropyl alcohol 70%	50313/50Wlo	1
Eigenherstellung	Isopropyl alcohol 70%	5114M-01080	1
C.Lange	Isopropyl alcohol 70%	50817/50La	1
Defektur / Wolf-Apotheke	Isopropyl alcohol 70%	50828/50Wlo	1
Eigen	Isopropyl alcohol 70%	5315I-01080	1
Defektur	Isopropyl alcohol 70%	5214A	1
Defektur	Isopropyl alcohol 70%	50907/50Si	1
Wolf- Apotheke / Defektur	Isopropyl alcohol 70%	50914/51Wlo	1
Claudia Lange	Isopropyl alcohol 70%	60620/50La	1
Defektur	Isopropyl alcohol 70%	60209/50Hk	1
Hedinger/AHD	Isopropyl alcohol 70%	53290	1
C.Lange	Isopropyl alcohol 70%	60307/51La	1
Fagron	Isopropyl alcohol 70%		1
Wolf-Apotheke	Isopropyl alcohol 70%	60623/50Dre	1
Claudia Lange	Isopropyl alcohol 70%	60704/50La	1
Claudia Lange	Isopropyl alcohol 70%	60620/51La	1
Defektur/Wolf-Apotheke	Isopropyl alcohol 70%	61215/50Dre	1
Martinus-Apotheke	Isopropyl alcohol 70%	A-030715-1D	1
Martinus-Apotheke	Isopropyl alcohol 70%	A-110716-2D	1
Martinus-Apotheke	Isopropyl alcohol 70%	A-241115-1D	1
Martinus-Apotheke	Isopropyl alcohol 70%	A-191214-1D	1
Martinus-Apotheke	Isopropyl alcohol 70%	A-150216-1D	1
Caelo	Isopropyl alcohol 70%	Ch14146701	1
Martinus-Apotheke	Isopropyl alcohol 70%	A-300714-1D	1
Martinus-Apotheke	Isopropyl alcohol 70%	A-200117-1D	1
Eigenherstellung	Isopropyl alcohol 70%	Eigenherstellung	2
Defektur	Isopropyl alcohol 70%		4
Rezeptur	Isopropyl alcohol 70%	Rezeptur	1
Neugereut Apotheke	Isopropyl alcohol 70%		2
Caelo	Isopropyl alcohol 70%		4

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Supplier	Substance	Batch	Spectra
Eigen	Isopropyl alcohol 70%		1
Eigenherstellung	Isopropyl alcohol 70%	9051212	1
Defektur	Isopropyl alcohol 70%	2/13	1
Caelo	Isopropyl alcohol 70%	2081202	1
Defektur	Isopropyl alcohol 70%	2/14	1
Defektur_JP_07012013	Isopropyl alcohol 70%	213A-07015	1
ASS	Isopropyl alcohol 70%	314A01080	1
Caelo	Isopropyl alcohol 70%	3091302	1
Neugereut Apotheke	Isopropyl alcohol 70%	214Q-01080	1
Defektur	Isopropyl alcohol 70%	514A	1
Rondell	Isopropyl alcohol 70%	414Q-07123	2
Defektur_JP_28012013	Isopropyl alcohol 70%	513A-07015	1
Gehe	Isopropyl alcohol 70%	53202	1
Noweda	Isopropyl alcohol 70%	5072012	1
hedinger	Isopropyl alcohol 70%	53236	2
Gehe	Isopropyl alcohol 70%	53215	1
Hedinger	Isopropyl alcohol 70%	53240	1
Hedinger	Isopropyl alcohol 70%	53241	3
Caelo	Isopropyl alcohol 70%	53241	2
Hedinger	Isopropyl alcohol 70%	53228	1
Hedinger	Isopropyl alcohol 70%	53226	1
Hedinger	Isopropyl alcohol 70%	53242	1
Hedinger	Isopropyl alcohol 70%	53250	1
Hedinger	Isopropyl alcohol 70%	53245	1
Phönix	Isopropyl alcohol 70%	53252	1
Euro OTC	Isopropyl alcohol 70%	53245	1
Hedinger	Isopropyl alcohol 70%	53253	2
Hedinger/Geilenkirchen	Isopropyl alcohol 70%	53262	1
Hedinger	Isopropyl alcohol 70%	53262	1
Hedinger	Isopropyl alcohol 70%	53259	1
Hedinger	Isopropyl alcohol 70%	53265	1
Hedinger	Isopropyl alcohol 70%	53255	1
Hedinger/AHD	Isopropyl alcohol 70%	53265	2
Hedinger/Geilenkirchen	Isopropyl alcohol 70%	53266	1
Hedinger	Isopropyl alcohol 70%	53267	1
Gehe	Isopropyl alcohol 70%	53268	1
Hedinger/AHD	Isopropyl alcohol 70%	53268	1
Defektur	Isopropyl alcohol 70%	7/14	1
Neugereut Apotheke	Isopropyl alcohol 70%	713M-01080	1
Hedinger/Sanacorp	Isopropyl alcohol 70%	53300	1
Hedinger/Hohe-Wart-Apot...	Isopropyl alcohol 70%	7082013/1	2
Apoth.E.Bartel	Isopropyl alcohol 70%	70545B/2	1
Hedinger	Isopropyl alcohol 70%	53274	1
Caelo	Isopropyl alcohol 70%	6041407	1
Caelo	Isopropyl alcohol 70%	7021307	1
Hirsch	Isopropyl alcohol 70%	714E-01080	1
Defektur	Isopropyl alcohol 70%	80114Iso70	1
Kastner	Isopropyl alcohol 70%	914I-01080	1
Defektur	Isopropyl alcohol 70%	9/13	1
Defektur_JP_25022013	Isopropyl alcohol 70%	913A-07015	1
Apolda	Isopropyl alcohol 70%	120214	1
Doppeleiche Apotheke	Isopropyl alcohol 70%	913A-01080	1
Hustadt Apotheke	Isopropyl alcohol 70%	120905	1
Caelo	Isopropyl alcohol 70%	121003	1
Defektur	Isopropyl alcohol 70%	100513Iso70	1
Caelo	Isopropyl alcohol 70%	12101301	1
Herstellung	Isopropyl alcohol 70%	110416P2	1
Hustadt Apotheke	Isopropyl alcohol 70%	121130	1
Caelo	Isopropyl alcohol 70%	12121306	1
Caelo	Isopropyl alcohol 70%	12136303	1

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Supplier	Substance	Batch	Spectra
Klenk	Isopropyl alcohol 70%	1214M-1080	1
Caelo	Isopropyl alcohol 70%	12278601	6
Caelo	Isopropyl alcohol 70%	12202801	2
Caelo	Isopropyl alcohol 70%	12136201	1
Caelo	Isopropyl alcohol 70%	12278704	2
Gehe/Phönix	Isopropyl alcohol 70%	12338001	2
Caelo	Isopropyl alcohol 70%	12278702	2
Caelo	Isopropyl alcohol 70%	12338001	1
Fagron	Isopropyl alcohol 70%	1234	2
Caelo	Isopropyl alcohol 70%	12338101	1
Caelo	Isopropyl alcohol 70%	130009002	2
Caelo	Isopropyl alcohol 70%	12338104	3
Caelo	Isopropyl alcohol 70%	130009003	1
Caelo	Isopropyl alcohol 70%	13008902	2
Caelo	Isopropyl alcohol 70%	13008903	2
Caelo	Isopropyl alcohol 70%	13009002	2
Stern-Defektur	Isopropyl alcohol 70%	130321004	1
Gutenberg-Apotheke	Isopropyl alcohol 70%	130206004	1
Caelo	Isopropyl alcohol 70%	13009003	1
Caelo	Isopropyl alcohol 70%	130205	1
Caelo	Isopropyl alcohol 70%	13031304	1
Defektur_EW_04062013	Isopropyl alcohol 70%	130604002	1
Gutenberg-Apotheke	Isopropyl alcohol 70%	130327003	1
Stern-Defektur	Isopropyl alcohol 70%	130425004	1
Defektur	Isopropyl alcohol 70%	130611/6	1
Gutenberg-Apotheke	Isopropyl alcohol 70%	130725001	1
Stern-Defektur	Isopropyl alcohol 70%	130703007	1
Stern-Defektur	Isopropyl alcohol 70%	130805002	1
Caelo	Isopropyl alcohol 70%	13092203	3
Gutenberg-Apotheke	Isopropyl alcohol 70%	130813006	1
Gutenberg-Apotheke	Isopropyl alcohol 70%	130912001	1
Caelo	Isopropyl alcohol 70%	13092201	1
Stern-Defektur	Isopropyl alcohol 70%	130927002	1
STERN	Isopropyl alcohol 70%	131202002	1
Phönix 12.06.2013	Isopropyl alcohol 70%	13092304	1
Caelo	Isopropyl alcohol 70%	13155403	3
Stern-Rezeptur	Isopropyl alcohol 70%	131015001	1
Stern-Defektur	Isopropyl alcohol 70%	131108001	1
Caelo	Isopropyl alcohol 70%	13155401	2
Stern-Defektur	Isopropyl alcohol 70%	131216005	1
Unisan	Isopropyl alcohol 70%	13155502	1
Caelo	Isopropyl alcohol 70%	13155503	6
Caelo	Isopropyl alcohol 70%	13217501	1
Caelo	Isopropyl alcohol 70%	13217603	2
Caelo	Isopropyl alcohol 70%	13217602	1
Caelo	Isopropyl alcohol 70%	13319405	2
Caelo	Isopropyl alcohol 70%	13337004	1
Caelo	Isopropyl alcohol 70%	13319502	2
Caelo	Isopropyl alcohol 70%	13363001	1
Phönix 13.01.2014	Isopropyl alcohol 70%	13319404	1
Caelo	Isopropyl alcohol 70%	13363003	2
Stern-Defektur	Isopropyl alcohol 70%	140116004	1
Stern-Defektur	Isopropyl alcohol 70%	140210001	1
Defektur	Isopropyl alcohol 70%	151113Iso70	1
Caelo	Isopropyl alcohol 70%	14101303	1
Caelo	Isopropyl alcohol 70%	15111304	1
Phonix	Isopropyl alcohol 70%	14026403	2
Caelo	Isopropyl alcohol 70%	14121205	1
Caelo	Isopropyl alcohol 70%	14026303	2
Defektur	Isopropyl alcohol 70%	16/13	1

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Supplier	Substance	Batch	Spectra
Caelo	Isopropyl alcohol 70%	1613q-01080	1
Caelo	Isopropyl alcohol 70%	15111305	1
Defektur	Isopropyl alcohol 70%	180413Iso70	1
Purren Apotheke	Isopropyl alcohol 70%	18043	1
Caelo	Isopropyl alcohol 70%	18061306	1
Caelo	Isopropyl alcohol 70%	18061307	1
Wensauer Apotheke	Isopropyl alcohol 70%		1
Caelo	Isopropyl alcohol 70%	20021414	1
Eigenherstellung	Isopropyl alcohol 70%	1823	2
Caelo	Isopropyl alcohol 70%	18101301	1
Caelo	Isopropyl alcohol 70%	20021415	1
hergestellt am 11.04.13	Isopropyl alcohol 70%	191012/925	1
Hirsch	Isopropyl alcohol 70%	1913E-01080	1
Herstellung in Apotheke	Isopropyl alcohol 70%	20120911	1
Defektur	Isopropyl alcohol 70%	200313Iso70	1
Caelo	Isopropyl alcohol 70%	20091302	1
DEFEKTUR	Isopropyl alcohol 70%	2013/08/14-1	1
DEFEKTUR	Isopropyl alcohol 70%	2013-09-16	1
Stern-Defektur	Isopropyl alcohol 70%	20130912	1
Herstellung in Apotheke	Isopropyl alcohol 70%	20130613	1
Defektur	Isopropyl alcohol 70%	210613Iso70	1
Herstellung in Apotheke	Isopropyl alcohol 70%	20130102	1
Stern-Defektur	Isopropyl alcohol 70%	20131022	1
Defektur	Isopropyl alcohol 70%	22/13	1
Caelo	Isopropyl alcohol 70%	22021303	1
Sonnen-Apotheke	Isopropyl alcohol 70%	210513H1	1
Herstellung in Apotheke	Isopropyl alcohol 70%	22042013	1
Caelo	Isopropyl alcohol 70%	22051301	1
Caelo	Isopropyl alcohol 70%	22051302	1
Caelo	Isopropyl alcohol 70%	221111205	1
Defektur	Isopropyl alcohol 70%	23712	1
Caelo	Isopropyl alcohol 70%	221111206	1
geiger	Isopropyl alcohol 70%	2213E-01080	1
Caelo	Isopropyl alcohol 70%	24081303	1
Defektur	Isopropyl alcohol 70%	250713Iso70	1
Caelo	Isopropyl alcohol 70%	24011405	1
Caelo	Isopropyl alcohol 70%	23041304	1
Winthrop	Isopropyl alcohol 70%	2600670T	1
Caelo	Isopropyl alcohol 70%	23041305	1
Caelo	Isopropyl alcohol 70%	24081207	1
Caelo	Isopropyl alcohol 70%	24101203	1
Caelo	Isopropyl alcohol 70%	2512A-01080	1
Winthrop	Isopropyl alcohol 70%	2600685T	1
GUMO/04.04.2013	Isopropyl alcohol 70%	2600726T	1
Defektur	Isopropyl alcohol 70%	27/13	1
Winthrop	Isopropyl alcohol 70%	2600681T	1
Eigenbedarf (Hergestel...	Isopropyl alcohol 70%	260613	1
Defektur	Isopropyl alcohol 70%	280513Iso70	1
Rondell Apotheke	Isopropyl alcohol 70%	2613Q-01080	2
eigene Herstellung	Isopropyl alcohol 70%	3013M-01080	1
Bombastus	Isopropyl alcohol 70%	2813Q-01080	1
Doppeleiche Apotheke	Isopropyl alcohol 70%	3013A-01080	1
Defektur	Isopropyl alcohol 70%	290813Iso70	1
Caelo	Isopropyl alcohol 70%	2600714T	1
Defektur	Isopropyl alcohol 70%	2812M-01080	1
Hedinger/Anzag	Isopropyl alcohol 70%	303006	1
Hedinger/Anzag	Isopropyl alcohol 70%	303007	2
Rondell Apotheke	Isopropyl alcohol 70%	3113M-07123	2
Germania Apo	Isopropyl alcohol 70%	315032	1
Gutenberg-Apotheke	Isopropyl alcohol 70%	3212I-01080	1

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Supplier	Substance	Batch	Spectra
rondell-Apotheke	Isopropyl alcohol 70%	3413M-07123	1
Defektur	Isopropyl alcohol 70%	37/13	1
Gutenberg-Apotheke	Isopropyl alcohol 70%	3812E-01080	1
Doppeleiche Apotheke	Isopropyl alcohol 70%	3413M-01080	1
Neugereut Apotheke	Isopropyl alcohol 70%	3531Q-01080	1
Defektur	Isopropyl alcohol 70%	3812	1
Apotheke am Holzweg	Isopropyl alcohol 70%	3912Y-01080	1
Doppeleiche Apotheke	Isopropyl alcohol 70%	4012M-01080	1
Igel Apotheke	Isopropyl alcohol 70%	3813E-01080	1
Gutenberg-Apotheke	Isopropyl alcohol 70%	4212A-01080	1
Gutenberg-Apotheke	Isopropyl alcohol 70%	4612I-01080	1
Eigen	Isopropyl alcohol 70%	4413A-01080	1
Euro OTC	Isopropyl alcohol 70%	4012Q-01080	1
Hirsch	Isopropyl alcohol 70%	4213E-01080	1
Hirsch	Isopropyl alcohol 70%	4413I-01080	1
Defektur	Isopropyl alcohol 70%	42/13	1
Caelo	Isopropyl alcohol 70%	4813E-01080	1
Doppeleiche Apotheke	Isopropyl alcohol 70%	4912M-01080	1
Neugereut Apotheke	Isopropyl alcohol 70%	4913M-01080	1
Defektur	Isopropyl alcohol 70%	5013A	1
Hirsch	Isopropyl alcohol 70%	5013Q-01080	1
Defektur	Isopropyl alcohol 70%	51/13	1
Defektur	Isopropyl alcohol 70%	53/12	1
Labor	Isopropyl alcohol 70%	7148	1
Defektur	Isopropyl alcohol 70%	58/13	1
Apotheke	Isopropyl alcohol 70%	8441	1
Caelo	Isopropyl alcohol 70%	8561	1
Apotheke	Isopropyl alcohol 70%	6710	1
Caelo	Isopropyl alcohol 70%	7581	1
Apotheke	Isopropyl alcohol 70%	8375	1
Sieg-Apotheke	Isopropyl alcohol 70%	661302027	1
Labor	Isopropyl alcohol 70%	8821	1
Labor	Isopropyl alcohol 70%	7988	1
Apotheke	Isopropyl alcohol 70%	9993	1
Martinus-Apotheke	Isopropyl alcohol 70%	A-131213-1D	2
Gehe/Wintrop	Isopropyl alcohol 70%	Ch2600715T	1
Labor	Isopropyl alcohol 70%	8885	1
Hedinger	Isopropyl alcohol 70%	B230715	1
Martinus-Apotheke	Isopropyl alcohol 70%	A-171013-1D	2
Apotheke	Isopropyl alcohol 70%	9385	1
Caelo	Isopropyl alcohol 70%	Eigenherstellung	1
Caolo	Isopropyl alcohol 70%	D07104T1	1
Eigenherstellung	Isopropyl alcohol 70%	eigene	2
Martinus-Apotheke	Isopropyl alcohol 70%	A-150314-1D	2
Hirsch	Isopropyl alcohol 70%	Die16041301	1
MAROS Arznei, Noweda	Isopropyl alcohol 70%		1
Defektur	Isopropyl alcohol 70%	H17042013B1	1
Caelo	Isopropyl alcohol 70%	H170315T1	1
selbst	Isopropyl alcohol 70%		1
Löwen Apotheke	Isopropyl alcohol 70%	H28122012P1	1
Caelo	Isopropyl alcohol 70%	H22062013H1	1
Caelo	Isopropyl alcohol 70%	H030315T1	1
Hedinger / Noweda	Isopropyl alcohol 70%	53266	1
Hedinger	Isopropyl alcohol 70%	53268	1
Sonnenberg-Apotheke	Isopropyl alcohol 70%	100214	1
Hedinger / Noweda	Isopropyl alcohol 70%	53267	1
Phönix	Isopropyl alcohol 70%	1217603	1
Wintrop	Isopropyl alcohol 70%	80616-12	1
Leyh Pharma	Isopropyl alcohol 70%	132021	1
Hedinger	Isopropyl alcohol 70%	1313E-01079	1

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Supplier	Substance	Batch	Spectra
Phönix	Isopropyl alcohol 70%	13217601	1
Caelo	Isopropyl alcohol 70%	13363104	1
Hetterich	Isopropyl alcohol 70%	140301	1
Defektur	Isopropyl alcohol 70%	1467/2014072920	1
Wintrop	Isopropyl alcohol 70%	2600863T	2
Wintrop AM GmbH/Anzag	Isopropyl alcohol 70%	2600754T	1
Wintrop	Isopropyl alcohol 70%	2600869t	1
winthrop	Isopropyl alcohol 70%	2600735T	1
Winthrop	Isopropyl alcohol 70%	2600706T	1
Wintrop	Isopropyl alcohol 70%	2600908t	1
Wintrop	Isopropyl alcohol 70%	2600969T	1
Defektur	Isopropyl alcohol 70%	3713Q-01080	1
Apotheke	Isopropyl alcohol 70%	4813Q-0180	1
Otto Fischar gmbh	Isopropyl alcohol 70%	4116045	1
Fischar	Isopropyl alcohol 70%	4116044	1

- 57 628 spectra from 332 *Apo-Ident* customers from a total of 19 482 batches from a further 328 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 *Isopropyl alcohol 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 *Isopropyl alcohol 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	160	0	34 184
Type B	0	440	0	63 154
Type C	0	789	24	57 628

The substance/substance group *Isopropyl alcohol 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.5963 %)	97.0480 % (> 96.6790 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31388	31388	0.00	82.21
31622	33105	6.38	82.64
31831	31388	3.96	80.37
33105	33105	0.00	78.04

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Isopropyl myristate
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30977-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Isopropyl myristate; Isopropylis myristas; Propylum myristinicum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Isopropyl myristate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Isopropyl myrist...	12171522	30977	80	1408077
Caelo	Isopropyl myrist...	13144311	31363	40	1412539
Euro OTC	Isopropyl myrist...	1303034-03	31530	40	20130502
Euro OTC	Isopropyl myrist...	1508035	31774	40	20150907*

Validation samples

A total of 156 379 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 *Isopropyl myristate*. These samples are listed above in the [calibration samples](#) section.
- 34 144 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 87 spectra of 4 reference samples from the substance/substance group *Isopropyl myristate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Isopropyl myristate	10119404	30193	7
Euro OTC	Isopropyl myristate	1303034-03	31530 [†]	20
Euro OTC	Isopropyl myristate	1508035	31774 [†]	20
Euro OTC	Isopropyl myristate	1608039	32776	40

- 63 507 spectra from a total of 1473 batches from further 439 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.

- 158 spectra from 68 *Apo-Ident* customers from 47 batches from the substance/substance group *Isopropyl myristate*.

*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.

[†]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*.

Supplier	Substance	Batch	Spectra
Euro OTC	Isopropyl myristate	1407015-03	10
Caelo	Isopropyl myristate	13144308	7
Euro OTC	Isopropyl myristate	1508035-01	8
Anzag	Isopropyl myristate	120100801	1
Euro OTC	Isopropyl myristate	1303034	1
Euro OTG	Isopropyl myristate	1303034-02	1
Euro/ Sanacorp	Isopropyl myristate	1303034-02	1
Euro OTC	Isopropyl myristate	1303034-02	19
Euroo/Phoenix	Isopropyl myristate	1303034-03	1
Euro OTC	Isopropyl myristate	1303034-03	9
Euro OTC	Isopropyl myristate	130303403	1
GEHE 26.11.2014	Isopropyl myristate	1303034-03	1
Fagron	Isopropyl myristate	13A17-B03-295774	2
Fagron	Isopropyl myristate	13A17-B05	1
Euro OTC	Isopropyl myristate	140701503	1
Euro OTC	Isopropyl myristate	1407015-01	3
Caelo	Isopropyl myristate	1407015-01	1
Euro/ Sanacorp	Isopropyl myristate	1407015-01	1
EuRho/Phönix	Isopropyl myristate	1407015-03	1
Euro OTC	Isopropyl myristate	1407015-02	2
Phoenix	Isopropyl myristate	1407015-03	2
Caelo	Isopropyl myristate	14155909	7
Caelo	Isopropyl myristate	14155902	1
Caelo	Isopropyl myristate	14155914	2
EuRho/Noweda	Isopropyl myristate	1417015-03	1
Euro/Phönix	Isopropyl myristate	1508035	1
Caelo	Isopropyl myristate	1508035-01	1
Wolf-Apotheke	Isopropyl myristate	1508035-02	1
Euro OTC	Isopropyl myristate	1508035-02	1
Caelo	Isopropyl myristate	15248304	1
Caelo	Isopropyl myristate	15438204	2
Caelo	Isopropyl myristate	15284807	1
Euro OTC	Isopropyl myristate	1608039-01	2
Caelo	Isopropyl myristate	30051502	1
Euro OTC	Isopropyl myristate	41140874	2
Euro OTC	Isopropyl myristate	3515Q-02898	1
Noweda	Isopropyl myristate	1106026-01	2
Euro OTC	Isopropyl myristate	968099	2
EuRho	Isopropyl myristate	1106026-01	1
Euro OTC	Isopropyl myristate	1106026-01	1
Caelo	Isopropyl myristate	11178415	1
Caelo	Isopropyl myristate	11178408	1
Noweda	Isopropyl myristate	120100801	1
Caesar&Loretz GmbH D-40...	Isopropyl myristate	1201008-01	1
Noweda	Isopropyl myristate	1201008-01	4
EuRho	Isopropyl myristate	1201008-01	1
Fiebig ek: 3,00EUR 31.08.12	Isopropyl myristate	1201008-01	1
Euro OTC	Isopropyl myristate	120100801	1
Euro OTC	Isopropyl myristate	1201008-01	3
Noweda	Isopropyl myristate	1212031-01	4
Anzag 1.03.13 ek:3,45EUR	Isopropyl myristate	121203101	2
Euro OTC	Isopropyl myristate	1212031-01	3
EuRho	Isopropyl myristate	12100801	1
Phönix	Isopropyl myristate	12171522	1
Noweda	Isopropyl myristate	12171511	1
EuRho/Phönix	Isopropyl myristate	1212031-01	1
Caelo	Isopropyl myristate	12171522	4
Caelo	Isopropyl myristate	12171518	1
Caelo	Isopropyl myristate	12248600	1
Caelo	Isopropyl myristate	13019902	5

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Supplier	Substance	Batch	Spectra
Caelo	Isopropyl myristate	12248601	1
Euro OTC	Isopropyl myristate	130133402	1
Caelo	Isopropyl myristate	13019910	3
Phönix, 18.07.2013	Isopropyl myristate	130303401	1
Euro OTC	Isopropyl myristate	1303034-01	4
Caelo	Isopropyl myristate	1303034-01	1
Caesar & Loretz GmbH	Isopropyl myristate	13019902	1
Phönix	Isopropyl myristate	13019910	1
AHD	Isopropyl myristate	1301992	1
Euro OTC	Isopropyl myristate	1407015	1

- 58 283 spectra from 332 *Apo-Ident* customers from a total of 20 046 batches from a further 328 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 *Isopropyl myristate* 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 *Isopropyl myristate* 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	34 144
Type B	0	87	0	63 507
Type C	0	155	3	58 283

The substance/substance group *Isopropyl myristate* 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 % (> 99.9690 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 93.1034 %)
Type C	100.0000 % (> 99.5963 %)	98.1013 % (> 96.2025 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30977	30977	0.00	30.47
31363	31363	0.00	34.25
31530	31774	1.40	32.88
31774	31774	0.00	33.41

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Isopropyl palmitate**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30868-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Isopropyl palmitate; Isopropylis palmitas; Propylum palmitinicum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Isopropyl palmitate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Isopropyl palmit...	12229109	30868	40	20120807
Bombastus	Isopropyl palmit...	284060	31268	40	20131119
Caelo	Isopropyl palmit...	14034806	31364	40	AR-15-FG-000372-01

Validation samples

A total of 156379 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 *Isopropyl palmitate*. These samples are listed above in the [calibration samples](#) section.
- 34224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 1 reference samples from the substance/substance group *Isopropyl palmitate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Isopropyl palmitate	16091706	32570	40

- 63554 spectra from a total of 1476 batches from further 439 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.

- 174 spectra from 95 *Apo-Ident* customers from 56 batches from the substance/substance group *Isopropyl palmitate*.

Supplier	Substance	Batch	Spectra
Bombastus	Isopropyl palmitate	299989	5
Caelo	Isopropyl palmitate	60092401	1
Bombastus	Isopropyl palmitate	266038	3
GEHE	Isopropyl palmitate	269359	1
Caelo	Isopropyl palmitate	11207309	2
Bombastus	Isopropyl palmitate	281766	5
Caelo	Isopropyl palmitate	11207301	5

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Supplier	Substance	Batch	Spectra
Caelo	Isopropyl palmitate	2081401	1
AHD	Isopropyl palmitate	14034801	1
Caelo	Isopropyl palmitate	14034806	4
Caelo	Isopropyl palmitate	14034807	9
Caelo	Isopropyl palmitate	14034801	1
Sanacorp	Isopropyl palmitate	14034807	1
Caelo	Isopropyl palmitate	14213111	1
Caelo	Isopropyl palmitate	15128803	8
Sanacorp	Isopropyl palmitate	15128803	1
Caelo	Isopropyl palmitate	15169701	6
Caelo	Isopropyl palmitate	15169705	1
Caelo	Isopropyl palmitate	16021504	1
Caelo	Isopropyl palmitate	16091701	5
Caelo	Isopropyl palmitate	16071504	1
Caelo	Isopropyl palmitate	281766	2
Bombastus	Isopropyl palmitate	284060	5
Brückenapotheke	Isopropyl palmitate	285604	1
Audor Pharma	Isopropyl palmitate	285604	1
Bombastus	Isopropyl palmitate	285604	4
Bombastus	Isopropyl palmitate	288083	5
Bombastus	Isopropyl palmitate	291043	3
Bombas über Sanacorp	Isopropyl palmitate	290363	1
Bombastus	Isopropyl palmitate	290363	3
Caelo	Isopropyl palmitate	293140	1
bombast/Px	Isopropyl palmitate	293140	1
Bombastus	Isopropyl palmitate	293140	7
Caelo	Isopropyl palmitate	291043	1
Bombastus	Isopropyl palmitate	297284	6
Fagron	Isopropyl palmitate	293140	1
Bombastus	Isopropyl palmitate	4613Q-02899	1
Bombastus	Isopropyl palmitate	302669	1
Bombastus	Isopropyl palmitate	3015I-02899	1
Bombastus	Isopropyl palmitate	262190	1
Bombastus	Isopropyl palmitate	269359	2
Hedinger	Isopropyl palmitate	271265	1
Bombastus	Isopropyl palmitate	271265	2
Bombastus	Isopropyl palmitate	272307	3
Sanacorp	Isopropyl palmitate	273823	1
Caelo	Isopropyl palmitate	273823	2
Bombastus	Isopropyl palmitate	273823	2
Caelo	Isopropyl palmitate	9324202	1
Caelo	Isopropyl palmitate	4061201	1
Fagron	Isopropyl palmitate	9G14-M08	2
Caelo	Isopropyl palmitate	12014106	2
Caelo	Isopropyl palmitate	12229109	2
Caelo	Isopropyl palmitate	13134903	3
Caelo	Isopropyl palmitate	131234905	1
Gehe	Isopropyl palmitate	12229112	1
Fiebig 21.08.13 EK5,60	Isopropyl palmitate	13134903	1
Caelo	Isopropyl palmitate	13134905	4
Noweda	Isopropyl palmitate	13134906	1
Caelo	Isopropyl palmitate	15071303	1
Caelo	Isopropyl palmitate	13134906	2
Caelo	Isopropyl palmitate	26021402	1
Caelo	Isopropyl palmitate	20210212-1	1
Bombastus	Isopropyl palmitate	26041301	1
Bombastus	Isopropyl palmitate	275014	7
Euro OTC	Isopropyl palmitate		1
Caelo	Isopropyl palmitate	25031302	1
Caelo	Isopropyl palmitate	17091205	1

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Supplier	Substance	Batch	Spectra
Bombastus	Isopropyl palmitate	276178	2
Bombastus	Isopropyl palmitate	277740	3
Anzag	Isopropyl palmitate	277740Bombastus	1
Bombastus	Isopropyl palmitate	279468	2
Bombastus	Isopropyl palmitate	281057	5
Caelo	Isopropyl palmitate	28111309	1
Phoenix	Isopropyl palmitate	281766	1
Bombastus	Isopropyl palmitate	60092401	1
Gutenberg-Apotheke	Isopropyl palmitate	285604	1

- 58 267 spectra from 332 *Apo-Ident* customers from a total of 20 037 batches from a further 328 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 *Isopropyl palmitate* 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 *Isopropyl palmitate* 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	34 224
Type B	0	40	0	63 554
Type C	0	170	4	58 267

The substance/substance group *Isopropyl palmitate* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.5963 %)	97.7011 % (> 95.9770 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30868	31364	5.10	16.25
31268	31364	2.71	19.09
31364	31364	0.00	19.80

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Juniper oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30711-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Juniper oil; Juniperi aetheroleum; Oleum juniperi e baccararum

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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
Caelo	Juniper oil	11379007	30711	40	1404599
Caelo	Juniper oil	13240811	31665	40	20130726

Validation samples

A total of 156 379 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 *Juniper oil*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 110 spectra of 4 reference samples from the substance/substance group *Juniper oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Juniper oil	13240807	31244	10
Caelo	Juniper oil	13240811	31665 [†]	20
Caelo	Juniper oil	15185205	32352	40
Caelo	Juniper oil	16160703	32918	40

- 63 484 spectra from a total of 1473 batches from further 439 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 12 *Apo-Ident* customers from 11 batches from the substance/substance group *Juniper oil*.

Supplier	Substance	Batch	Spectra
Caelo	Juniper oil	13240802	3

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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
Caelo	Juniper oil	14115802	1
Caelo	Juniper oil	11379006	1
Caelo	Juniper oil	15141302	1
Caelo	Juniper oil	111275	1
Caelo	Juniper oil	11379003	1
Caelo	Juniper oil	11379007	1
Caelo	Juniper oil	11379012	2
Sanacorp	Juniper oil	11379012	1
Caelo	Juniper oil	11379017	1
Caelo	Juniper oil	18121306	1
Caelo	Juniper oil	12322707	1

- 58 426 spectra from 332 *Apo-Ident* customers from a total of 20 082 batches from a further 328 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	80	0	34 264
Type B	0	68	42	63 484
Type C	0	14	1	58 426

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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9710 %)	61.8182 % (> 59.0909 %)
Type C	100.0000 % (> 99.5969 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30711	30711	0.00	28.16
31665	30711	15.65	24.69

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Lactic acid**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30021-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lactic acid; Acidum lacticum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Lactic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lactic acid	12142108	30734	39	AR-14-FG-012230-01
Caelo	Lactic acid	13317311	31436	40	20131011

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 79 spectra of 2 reference samples from the substance/substance group *Lactic acid*. These samples are listed above in the [calibration samples](#) section.
- 34 265 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Lactic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lactic acid	90646219	30021	40
Caelo	Lactic acid	13317311	31436 [†]	20

- 63 534 spectra from a total of 1475 batches from further 439 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.

- 321 spectra from 178 *Apo-Ident* customers from 78 batches from the substance/substance group *Lactic acid*.

Supplier	Substance	Batch	Spectra
Caelo	Lactic acid	11179209	1
Caelo	Lactic acid	11179217	7
Caelo	Lactic acid	13317308	8

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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
Gutenberg-Apotheke	Lactic acid	13317303	1
Caelo	Lactic acid	13317313	5
Caelo	Lactic acid	14112112	4
A.H.D.	Lactic acid	15150402	1
Caelo	Lactic acid	15150401	3
Caelo	Lactic acid	13317315	4
Caelo	Lactic acid	15150410	8
Caelo	Lactic acid	12142102	8
Caelo	Lactic acid	15308608	6
Caelo	Lactic acid	15150413	5
Caelo	Lactic acid	15150421	5
Caelo	Lactic acid	13020203	6
Caelo	Lactic acid	12142112	12
Caelo	Lactic acid	13317301	28
Caelo	Lactic acid	13020201	16
GEHE	Lactic acid	21021180/2	1
Caelo	Lactic acid	11179207	3
Caelo	Lactic acid	13020212	1
Caelo	Lactic acid	13317303	2
Caelo	Lactic acid	12142162	1
Caelo	Lactic acid	13317307	13
Caesar & Loretz GmbH	Lactic acid	13317308	1
Caelo	Lactic acid	13317311	15
Sanacorp	Lactic acid	13317311	1
Caelo/Kehr	Lactic acid	13317312	1
Caelo	Lactic acid	14112106	3
Caelo	Lactic acid	13317393	1
Caelo	Lactic acid	14112107	8
Caesar & Loretz GmbH Hi...	Lactic acid	14112112	1
Euro OTC	Lactic acid	14112112	1
Noweda 18.05.2015	Lactic acid	141121119	1
Caesar & Loretz GmbH	Lactic acid	14112107	1
Caelo	Lactic acid	14112114	3
Caelo	Lactic acid	14112115	5
Phoenix Goettin	Lactic acid	14112115	1
Caelo	Lactic acid	14112116	2
Caelo	Lactic acid	14112119	7
Caelo	Lactic acid	1510402	1
Caelo	Lactic acid	1510421	1
Caesar&Loretz/Noweda	Lactic acid	15150402	1
Caelo	Lactic acid	15150402	7
Rondell Apotheke	Lactic acid	15150402	1
Caelo	Lactic acid	15150405	2
Noweda	Lactic acid	15150410	1
Caelo	Lactic acid	15150418	1
Caelo	Lactic acid	15308601	6
Caelo	Lactic acid	2182	1
Caelo	Lactic acid	17031502	1
Caelo	Lactic acid	2101202	1
Caelo	Lactic acid	5031301	1
Caelo	Lactic acid	10323202	1
Caelo	Lactic acid	408Q-01034	1
Caelo	Lactic acid	9064607	1
Caelo	Lactic acid	913Q-01034	1
Caelo	Lactic acid	10/AKD1	1
Caelo	Lactic acid	11179201	1
Caelo	Lactic acid	11111644	1
Gehe	Lactic acid	11179217	1
v.d.l	Lactic acid	11179207	1
Gehe	Lactic acid	11179207	1

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Supplier	Substance	Batch	Spectra
Caelo	Lactic acid	11179214	1
Caelo	Lactic acid	12142101	10
Caelo	Lactic acid	12142104	2
Caelo	Lactic acid	12142108	9
Caelo	Lactic acid	12142109	2
Phoenix	Lactic acid	1214212	1
AHD, 25.11.13	Lactic acid	1302011	1
Phönix, 21.03.2013	Lactic acid	13020201	1
Sanacorp	Lactic acid	13020201	1
Noweda	Lactic acid	13020208	1
Caelo	Lactic acid	13020208	6
Gehe	Lactic acid	13020208	1
Unisan	Lactic acid	13020208	1
Caelo	Lactic acid	13020211	15
Caelo	Lactic acid	1302021	1
Caesar&Loretz GmbH/Anzag	Lactic acid	13020211	1
Caelo	Lactic acid	130360	1
Caelo	Lactic acid	1309211034	1
Caelo	Lactic acid	13317304	3
Caelo	Lactic acid	133173082x	1
Sanacorp	Lactic acid	13317307	1
Caesar&Loretz,AHC	Lactic acid	13317309	1
Caelo	Lactic acid	13317309	1
Euro OTC	Lactic acid	1503086-03	1
Phoenix	Lactic acid	15308608	1
Caesar&Loretz GmbH	Lactic acid	15308601	1
Phoenix	Lactic acid	15308613	1
Caelo	Lactic acid	16121-01034	1
Rondell Apotheke	Lactic acid	15308613	1
Caelo	Lactic acid	15308609	1
Caelo	Lactic acid	15308613	2
Caelo	Lactic acid	16144201	3
Caelo	Lactic acid	2014U-01034	1
	Lactic acid	71449138	2
Caelo	Lactic acid	20221110-4	1
Caelo	Lactic acid	A-220413-3	1
Caelo	Lactic acid	2710Q-01034	1
Caelo	Lactic acid	90646369	1
Caelo	Lactic acid	81302029	1
Caelo	Lactic acid	A-310513-1	1
Noweda	Lactic acid	81302139	1

- 58 120 spectra from 332 *Apo-Ident* customers from a total of 20 014 batches from a further 328 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 *Lactic 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 *Lactic 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	79	0	34 265
Type B	0	56	4	63 534
Type C	0	269	52	58 120

The substance/substance group *Lactic 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 % (> 99.9692 %)	100.0000 % (> 92.4051 %)
Type B	100.0000 % (> 99.9711 %)	93.3333 % (> 88.3333 %)
Type C	100.0000 % (> 99.5963 %)	83.8006 % (> 82.8660 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30734	30734	0.00	78.24
31436	30734	7.07	76.37

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Lanette® ointment (conserved)**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30499-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lanette® ointment (conserved); Unguentum Lanette®

Special notes

When selecting the *Lanette® ointment (conserved)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Lanette® ointment (conserved)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lanette® ointmen...	13257301	31166	40	1402587
Caelo	Lanette® ointmen...	13257301	31225	40	1403113
Caelo	Lanette® ointmen...	13393001	31454	30	20131206
Caelo	Lanette® ointmen...	153481	31913	40	20151111*
Caelo	Lanette® ointmen...	153482	31914	40	20151111*
Caelo	Lanette® ointmen...	160894	32093	40	20160318*
Caelo	Lanette® ointmen...	162580	32500	40	20160920*

Validation samples

A total of 156379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 270 spectra of 7 reference samples from the substance/substance group *Lanette® ointment (conserved)*. These samples are listed above in the [calibration samples](#) section.
- 34074 spectra from a total of 792 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 510 spectra of 14 reference samples from the substance/substance group *Lanette® ointment (conserved)*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lanette® ointment (conserved)	11256001	30423	40
Caelo	Lanette® ointment (conserved)	90249059	30437	40
Caelo	Lanette® ointment (conserved)	11367801	30473	40
Caelo	Lanette® ointment (conserved)	11367901	30499	40
Caelo	Lanette® ointment (conserved)	12223801	30777	40
Caelo	Lanette® ointment (conserved)	13393001	31454 [†]	10
Caelo	Lanette® ointment (conserved)	153481	31913 [†]	20
Caelo	Lanette® ointment (conserved)	153482	31914 [†]	20
Caelo	Lanette® ointment (conserved)	153483	31915	60
Caelo	Lanette® ointment (conserved)	162580	32501	40
Caelo	Lanette® ointment (conserved)	162581	32502	40
Caelo	Lanette® ointment (conserved)	162581	32503	40
Caelo	Lanette® ointment (conserved)	162582	32504	40
Caelo	Lanette® ointment (conserved)	162582	32505	40

- 63084 spectra from a total of 1465 batches from further 439 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the

*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.

[†]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*.

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.

- 259 spectra from 77 *Apo-Ident* customers from 70 batches from the substance/substance group *Lanette® ointment (conserved)*.

Supplier	Substance	Batch	Spectra
Caelo	Lanette® ointment (conserved)	13393001	12
Caelo	Lanette® ointment (conserved)	14277401	14
Caelo	Lanette® ointment (conserved)	14277101	3
Caelo	Lanette® ointment (conserved)	15048801	1
Caelo	Lanette® ointment (conserved)	14277301	2
Caelo	Lanette® ointment (conserved)	15048901	10
Caelo	Lanette® ointment (conserved)	15049001	8
Caelo	Lanette® ointment (conserved)	15095902	2
Caesar & Loretz GmbH / ...	Lanette® ointment (conserved)	15211301	1
Caelo	Lanette® ointment (conserved)	15211301	9
Caelo	Lanette® ointment (conserved)	15211201	2
Caelo	Lanette® ointment (conserved)	152114021	1
Caesar & Loretz GmbH	Lanette® ointment (conserved)	15348201	1
Caelo	Lanette® ointment (conserved)	15211401	2
Caelo	Lanette® ointment (conserved)	15348301	3
Caelo	Lanette® ointment (conserved)	16089401	14
Phoenix	Lanette® ointment (conserved)	16089402	2
Caelo	Lanette® ointment (conserved)	16089402	5
Caelo	Lanette® ointment (conserved)	13257301	12
Caelo	Lanette® ointment (conserved)	16089404	1
Caelo	Lanette® ointment (conserved)	8041502	1
Caelo	Lanette® ointment (conserved)	16184702	2
Caelo	Lanette® ointment (conserved)	16188701	2
Caelo	Lanette® ointment (conserved)	19082015C	1
Caelo	Lanette® ointment (conserved)	13392701	8
Caelo	Lanette® ointment (conserved)	14089601	2
Caelo	Lanette® ointment (conserved)	14089501	5
Phoenix	Lanette® ointment (conserved)	14089501	1
AHD	Lanette® ointment (conserved)	14089801	1
Caelo	Lanette® ointment (conserved)	14089801	8
Sanacorp	Lanette® ointment (conserved)	14089801	1
Caelo	Lanette® ointment (conserved)	1420061	1
Caelo	Lanette® ointment (conserved)	14200601	3
Caelo	Lanette® ointment (conserved)	14221601	2
Caelo	Lanette® ointment (conserved)	16071402	1
Caelo	Lanette® ointment (conserved)	40/AKD2	1
Caelo	Lanette® ointment (conserved)	11367901	4
Caelo	Lanette® ointment (conserved)	12081301	6
Caelo	Lanette® ointment (conserved)	12223701	2
Caelo	Lanette® ointment (conserved)	1222380	1
Caelo	Lanette® ointment (conserved)	1208131	1
Caelo	Lanette® ointment (conserved)	12313101	5
Caelo	Lanette® ointment (conserved)	13046601	4
Caelo	Lanette® ointment (conserved)	12223801	7
Caelo	Lanette® ointment (conserved)	1231302	1
GEHE	Lanette® ointment (conserved)	13046701	1
Caelo	Lanette® ointment (conserved)	13046701	15

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Supplier	Substance	Batch	Spectra
Alliance	Lanette [®] ointment (conserved)	13046701	1
Caelo	Lanette [®] ointment (conserved)	13177501	10
Caelo	Lanette [®] ointment (conserved)	13046802	4
Caelo	Lanette [®] ointment (conserved)	13234007	1
Caelo	Lanette [®] ointment (conserved)	13257501	11
Caelo	Lanette [®] ointment (conserved)	20021309	1
Caelo	Lanette [®] ointment (conserved)	20310812-5	1
Caelo	Lanette [®] ointment (conserved)	20110712-3	1
Caelo	Lanette [®] ointment (conserved)	28111311	1
Caelo	Lanette [®] ointment (conserved)	11367801	1
Caelo	Lanette [®] ointment (conserved)	613Q-03211	1
Anzag,31.06.2012	Lanette [®] ointment (conserved)	12081301	2
Phönix	Lanette [®] ointment (conserved)	12223701	1
Caelo	Lanette [®] ointment (conserved)	12170301	1
Caelo	Lanette [®] ointment (conserved)	12313102	2
Caelo	Lanette [®] ointment (conserved)	1277	1
Caelo	Lanette [®] ointment (conserved)	130456601	1
Alliance Healthcare/Lam...	Lanette [®] ointment (conserved)	13046601	1
Caelo	Lanette [®] ointment (conserved)	13191201	5
gehe	Lanette [®] ointment (conserved)	13177501	1
Caelo	Lanette [®] ointment (conserved)	13257402	1
Caelo	Lanette [®] ointment (conserved)	13392901	3
Caelo	Lanette [®] ointment (conserved)	1391201	1
Caelo	Lanette [®] ointment (conserved)	35151-03211	1
Caelo	Lanette [®] ointment (conserved)	U-150513-3	1
Anzah / Henry lammotte	Lanette [®] ointment (conserved)	13257501	1
Caelo	Lanette [®] ointment (conserved)	14277201	2
Caelo	Lanette [®] ointment (conserved)	15211102	1
Caelo	Lanette [®] ointment (conserved)	15348202	1
Caelo	Lanette [®] ointment (conserved)	16188801	1
Caelo	Lanette [®] ointment (conserved)	12312101	1
Caelo	Lanette [®] ointment (conserved)	12313001	1
Caelo	Lanette [®] ointment (conserved)	13046501	2
Caelo	Lanette [®] ointment (conserved)	12312901	1
Caelo	Lanette [®] ointment (conserved)	13177301	1

- 58 182 spectra from 332 *Apo-Ident* customers from a total of 20 025 batches from a further 328 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 *Lanette[®] ointment (conserved)* 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 *Lanette[®] ointment (conserved)* 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	270	0	34 074
Type B	0	506	4	63 084
Type C	0	201	58	58 182

The substance/substance group *Lanette[®] ointment (conserved)* 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 % (> 99.9689 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9710 %)	99.2157 % (> 98.6275 %)
Type C	100.0000 % (> 99.5963 %)	77.6062 % (> 76.4479 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31166	31166	0.00	24.09
31225	31225	0.00	25.48
31454	31225	3.08	23.33
31913	31913	0.00	23.87
31914	31914	0.00	29.49
32093	32093	0.00	25.58
32500	32500	0.00	24.36

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Lanolin**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30013-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lanolin; Lanolinum; Unguentum adipis lanae

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Lanolin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lanolin	13062501	31003	40	20130226
Caelo	Lanolin	14032001	31439	40	AR-15-FG-008283-01
Caelo	Lanolin	15255201	31746	40	20150727
Fagron	Lanolin	15G02-T11-024155	31794	40	AR-16-FG-004053-01
Bombastus	Lanolin	294969	31795	40	20150611
Caelo	Lanolin	15405502	31798	40	20151130
Caelo	Lanolin	163026	32863	40	20161028*

Validation samples

A total of 156379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Lanolin*. These samples are listed above in the [calibration samples](#) section.
- 34064 spectra from a total of 791 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 415 spectra of 12 reference samples from the substance/substance group *Lanolin*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lanolin	90870149	30013	30
Henry Lamotte	Lanolin	4922600	30163	65
Bombastus	Lanolin	258524	30228	40
Henry Lamotte	Lanolin	5264900	30922	40
Caelo	Lanolin	15255201	31746 [†]	20
Fagron	Lanolin	15G02-T11-024155	31794 [†]	20
Bombastus	Lanolin	294969	31795 [†]	20
Caelo	Lanolin	15405502	31798 [†]	20
Caelo	Lanolin	163022	32859	40
Caelo	Lanolin	163023	32860	40
Caelo	Lanolin	163024	32861	40
Caelo	Lanolin	163025	32862	40

- 63179 spectra from a total of 1465 batches from further 439 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](#).

*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.

[†]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*.

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.

- 950 spectra from 234 *Apo-Ident* customers from 228 batches from the substance/substance group *Lanolin*.

Supplier	Substance	Batch	Spectra
Caelo	Lanolin	14165601	29
Caelo	Lanolin	12193702	2
Caelo	Lanolin	12194201	4
Caelo	Lanolin	14165901	21
Bombastus	Lanolin	266983	1
Bombastus	Lanolin	264723	2
Bombastus	Lanolin	264721	1
Bombastus	Lanolin	9/14	1
Bombastus	Lanolin	270439	1
Bombastus	Lanolin	270443	1
Caelo	Lanolin	213Q-01765	1
Caelo	Lanolin	7071205	1
Caelo	Lanolin	713I-01765	1
Caelo	Lanolin	8071503	1
Caelo	Lanolin	9041401	1
Caelo	Lanolin	9011406	1
Caelo	Lanolin	10358301	1
Caelo	Lanolin	11011404	1
Phönix	Lanolin	11113902	1
DAB 2008	Lanolin	11281701	1
Caelo	Lanolin	11281702	2
Euro OTC	Lanolin	11281901	2
Caelo	Lanolin	11282001	3
Gehe	Lanolin	11282001	1
Anzag	Lanolin	11315101	1
Caelo	Lanolin	11315101	4
Caelo	Lanolin	11315102	3
Fagron	Lanolin	11k18-t01	1
Caesar & Loretz GmbH, 4...	Lanolin	12037101	1
Caelo	Lanolin	12037101	7
Caelo	Lanolin	12037002	1
Phönix Gotha	Lanolin	12037101	1
Caelo	Lanolin	12037301	2
VDL	Lanolin	12037301	1
Caelo	Lanolin	12037401	5
Caelo	Lanolin	12065101	5
Noweda	Lanolin	12065101	1
Caelo	Lanolin	12065102	3
VDL	Lanolin	12065101/32	1
Caelo	Lanolin	12193701	21
Gehe	Lanolin	12193701	1
Sanacorp	Lanolin	12193701	1
Caesar & Loretz GmbH	Lanolin	12193701	1
Caesar & Loretz GmbH	Lanolin	12193701	1
Caelo	Lanolin	12193901	12
Anzag/	Lanolin	12193901	1
Phönix Gotha	Lanolin	12193901	1
Großhandel	Lanolin	12193901	1
Caesar & Loretz GmbH, 4...	Lanolin	12260301	1
Caelo	Lanolin	12260301	5
Caelo	Lanolin	12260302	3
Caelo	Lanolin	12308601	8

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Supplier	Substance	Batch	Spectra
Caelo	Lanolin	12308801	2
Caelo	Lanolin	12308802	20
Phönix Gotha	Lanolin	12308802	1
Sanacorp	Lanolin	12308801	1
Sanacorp	Lanolin	12308802	2
Erika apotheke	Lanolin	12308802	1
Caelo	Lanolin	123456	1
Fagron	Lanolin	12C06-T02	1
Bombastus	Lanolin	124967	1
Fagron	Lanolin	12C06-T03	1
Fagron	Lanolin	12E22-T04	4
Phönix 08.01.13	Lanolin	12E22-T04	1
Fagron	Lanolin	12E22-T07	1
Kehr	Lanolin	12H01-T01	1
Fagron	Lanolin	12E22-T06	1
Caelo	Lanolin	12H01-T01	1
Fagron	Lanolin	12H01-T01	3
Caelo	Lanolin	12H01-T02	1
Fagron	Lanolin	12H01-T04	2
Caelo	Lanolin	13062401	12
Phoenix 22.03.13	Lanolin	13062401	2
Fagron	Lanolin	12H01-T03	1
Phoenix	Lanolin	12H01-T03	1
Caesar & Loretz GmbH, 4...	Lanolin	13062401	1
Phönix Gotha	Lanolin	13062401	2
Großhandel	Lanolin	13062401	1
Alliance Healthcare	Lanolin	13062401	1
Phönix	Lanolin	13062401	1
Sanacorp	Lanolin	13062401	1
Caelo	Lanolin	13062501	12
Fagron	Lanolin	13062501	1
Gehe	Lanolin	13062501	2
Caelo	Lanolin	13062602	4
Caelo	Lanolin	13062701	8
Caelo	Lanolin	13062801	2
Alliance	Lanolin	13102802	1
Caelo	Lanolin	13102802	22
Caelo	Lanolin	1306501	1
Noweda	Lanolin	13102802	1
Bombastus	Lanolin	13173601	1
phönix	Lanolin	13121001	1
Caelo	Lanolin	1310802	1
Caelo	Lanolin	13227601	20
Gehe	Lanolin	13227601	1
Caelo	Lanolin	13227602	5
Caelo	Lanolin	13227701	14
Noweda	Lanolin	13227701	1
Caelo	Lanolin	13227801	7
Phönix Gotha	Lanolin	13227701	2
Caelo	Lanolin	13326501	19
GEHE 12.03.2014	Lanolin	13326501	2
Caelo	Lanolin	13326502	4
Gehe	Lanolin	13326601	1
Caelo	Lanolin	13326601	7
Krieger	Lanolin	133266012x	1
Caelo	Lanolin	13326701	25
Großhandel	Lanolin	13326701	1
Phönix	Lanolin	13326701	1
Caelo	Lanolin	13345902	18
Caelo	Lanolin	13345901	1

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Supplier	Substance	Batch	Spectra
Caelo	Lanolin	133326701	1
Noweda	Lanolin	13345902	1
Fagron	Lanolin	13804T21001085	1
Fagron	Lanolin	13B04-T20-001084	2
Fagron	Lanolin	13B04-T20-00108	1
Fagron	Lanolin	13804-T22-0002	1
Gehe	Lanolin	13B04-T20-001084	1
fargon	Lanolin	13B04-T20-001084	1
phönix	Lanolin	13B04-T20-001084	1
Fagron	Lanolin	13B04-T20-0010B4	1
Fagron	Lanolin	13B04-T21-001085	3
Fagron	Lanolin	13B04-T22-001078	2
Fagron	Lanolin	13B12-T01-001087	2
Fagron	Lanolin	13E07-T18-003392	1
Fagron	Lanolin	13E0760-0002	1
Caelo	Lanolin	13E07-T20-003399	2
Fagron	Lanolin	13E07-T20-003401	2
Fagron	Lanolin	13E07-T21-003404	1
Fagron	Lanolin	13E07-Trg-oo3395	1
Fagron	Lanolin	13E07-T22-003407	1
Fagron	Lanolin	13H13-T08006173	1
Fagron	Lanolin	13H13-T08-006173	2
Fagron	Lanolin	13H13T11-006183	1
Fagron	Lanolin	13H13-12	1
Fagron	Lanolin	13H13T11006184	1
Fagron	Lanolin	13H13-T12-006187	3
Fagron	Lanolin	13H13-To9-006176	1
Caelo	Lanolin	13H13-To8-006173	1
Caelo	Lanolin	14032001	18
Caelo	Lanolin	14011304	1
GEHE 14.04.2014	Lanolin	14032001	2
Caesar & Loretz GmbH	Lanolin	14032001	1
Gehe	Lanolin	14032001	1
Gehe 29.07.14	Lanolin	14032001	1
Caelo	Lanolin	14032101	15
Großhandel	Lanolin	14032101	1
Phönix Gotha	Lanolin	14032101	1
Caelo	Lanolin	14032201	3
Caelo	Lanolin	14032301	10
Noweda	Lanolin	14032301	1
Caelo	Lanolin	14032302	2
Caelo	Lanolin	14032401	3
Sanacorp	Lanolin	14032301	1
Caelo	Lanolin	14101306	1
Phönix	Lanolin	14165601	1
Bombastus	Lanolin	14165601	1
Gehe	Lanolin	14165601	2
Caesar & Loretz GmbH	Lanolin	14165601	1
Caelo	Lanolin	14165701	2
Sanacorp	Lanolin	14165901	1
Phönix Gotha	Lanolin	14165901	2
Caelo	Lanolin	14166001	7
Fagron	Lanolin	14166001	1
Caelo	Lanolin	14333602	18
Caelo	Lanolin	1433001	1
Caesar&lorenz,Phoenix	Lanolin	14333602	1
Caelo	Lanolin	14333701	4
Caelo	Lanolin	14333901	4
Caelo	Lanolin	14334001	16
Phönix Gotha	Lanolin	14334001	1

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Supplier	Substance	Batch	Spectra
Caelo	Lanolin	1433602	3
ANZAG 01.01.143	Lanolin	14a06-t01-009011	1
Fagron	Lanolin	14A06T01009011	1
Fagron	Lanolin	14A06-T01-009011	3
Caelo	Lanolin	14A06-T01-009011	1
Fagron	Lanolin	14A06T02	3
Fagron	Lanolin	14A06T02009014	1
Fagron	Lanolin	14A06-T03-009017	1
Fagron	Lanolin	14A06-T02-009014	1
Alliance health 12.01.15	Lanolin	14A06-T05-0002	1
Fagron	Lanolin	14A06-T06-009028	1
GEHE 26.11.2014	Lanolin	14A06-T04-009021	1
Fagron	Lanolin	14E06-T07	1
Fagron	Lanolin	14E06T07	1
Fagron	Lanolin	14E06-T07-012186	3
Fagron	Lanolin	14E06-T09-012194	3
Fagron	Lanolin	14E06-T11-012200	1
GEHE	Lanolin	14K11-T03-016984	1
Caelo	Lanolin	14K11-T01-016976	2
Fagron	Lanolin	14K11-T03-016984	1
Caelo	Lanolin	15024102	16
Fagron	Lanolin	14K11-T01-016976	1
Caelo	Lanolin	15024003	1
Caesar & Loretz GmbH	Lanolin	15024102	1
Phönix Gotha	Lanolin	15024201	2
Caelo	Lanolin	15024201	20
Caelo	Lanolin	15024301	2
Caelo	Lanolin	1515Q-01765	1
Caelo	Lanolin	15045502	1
Caelo	Lanolin	15193401	7
Phönix	Lanolin	15193401	1
Phönix Gotha	Lanolin	15193401	1
Caelo	Lanolin	15193501	11
Caelo	Lanolin	1525501	1
Caelo	Lanolin	15255201	10
Caelo	Lanolin	15255202	12
Caelo	Lanolin	15255301	3
Caelo	Lanolin	15255601	2
Caelo	Lanolin	15255501	1
Caelo	Lanolin	15405501	9
Caelo/ AHD	Lanolin	15405501	1
Alliance H.	Lanolin	15405501	1
Noweda	Lanolin	15405501	1
caesar&lorenz,Phönix	Lanolin	15405502	1
Caelo	Lanolin	15405502	17
Caelo	Lanolin	15405601	12
Caelo	Lanolin	15c1903020815	1
Fargron/Noweda	Lanolin	15C19-T01-020809	1
Caelo	Lanolin	15405801	2
Caelo	Lanolin	15C19-T01-020809	2
Noweda	Lanolin	15C19-T02-020812	1
Fagron	Lanolin	15c19-t02-020812	1
Fagron	Lanolin	15C19T03	1
Fagron	Lanolin	15C19-T03-020815	2
Caelo	Lanolin	16054602	4
Caelo	Lanolin	16011501	1
Fagron	Lanolin	15c19-t05-020821	1
Gehe	Lanolin	16054602	1
Caelo	Lanolin	16054701	4
Caelo	Lanolin	16054801	11

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Supplier	Substance	Batch	Spectra
Cealo/AHD	Lanolin	16054801	2
Cealo	Lanolin	16054901	13
Phönix	Lanolin	16054901	1
Phoenix	Lanolin	16054901	2
Euro OTC	Lanolin	16054901	2
Cealo	Lanolin	16064901	1
Phoenix	Lanolin	16189401	1
Caesar & Loretz	Lanolin	16189401	1
Cealo	Lanolin	16189401	3
Caesar & Loretz GmbH Hi...	Lanolin	16189401	1
Cealo	Lanolin	16189501	3
Cealo	Lanolin	16189402	1
Anzag	Lanolin	16189501	1
Cealo	Lanolin	16302202	1
Cealo	Lanolin	16189701	1
Phoenix	Lanolin	16302301	1
Cealo	Lanolin	16302301	4
Cealo	Lanolin	16302401	3
Cealo	Lanolin	17082015D	1
Fagron	Lanolin	16G01-T04-034850	1
Fagron	Lanolin	16G01-T05-034853	1
Cealo	Lanolin	20240912-1	1
Cealo	Lanolin	23326501	1
Euro OTC	Lanolin	260416v1	1
Cealo	Lanolin	26061401	1
Bombstus	Lanolin	273293	1
Bombastus	Lanolin	274413	2
Bombastus	Lanolin	274412	1
AHD , 05.09.13	Lanolin	274414	1
Bombastus	Lanolin	274414	1
Bombastus	Lanolin	276824	1
Bombastus	Lanolin	277970	4
Bombastus	Lanolin	277969	1
Bombastus	Lanolin	277967	2
Bombastus	Lanolin	280111	3
Raben-Apotheke Mildenau	Lanolin	282976	1
AHD, 08.11.13	Lanolin	280111	1
Bombastus	Lanolin	285097	3
Bombastus	Lanolin	286688	1
Bombastus	Lanolin	285096	2
Bombastus	Lanolin	286691	3
Bombastus	Lanolin	286690	1
Rabenapotheke	Lanolin	288634	2
Bombastus	Lanolin	288636	1
Bombastus	Lanolin	288637	3
Bombastus	Lanolin	290885	2
Bombastus	Lanolin	292904	1
Bombastus	Lanolin	292906	2
Bombastus	Lanolin	297583	1
Bombastus	Lanolin	294967	2
phönix	Lanolin		1
Cealo	Lanolin	31121301	1
Bombastus	Lanolin	302807	1
Bombastus	Lanolin	300144	1
Cealo	Lanolin	3613A-01765	1
Cealo	Lanolin	4413M01765	1
phönix	Lanolin	34/AKD2	1
Cealo	Lanolin	5113A-01765	1
Sanacorp	Lanolin	34/AKD1	1
Lamotte/Noweda	Lanolin	5152000	1

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Supplier	Substance	Batch	Spectra
Caelo	Lanolin	5211Q-01765	1
anzag, 05.11.2012	Lanolin	5152000	1
Henry Lamotte Oils	Lanolin	5264900	1
Anzag	Lanolin	5264900	1
Lamotte/Noweda	Lanolin	5264900	1
Anzag/Henry Lamotte	Lanolin	5264900	1
Henry Lamotte Oils GmbH...	Lanolin	5264900	1
Anzag 10.04.13	Lanolin	5264900	1
Phönix	Lanolin	5316400	1
Henry Lamotte Oils/anzag	Lanolin	5375500	3
Alliance Healthcare	Lanolin	5375500	1
Henry	Lanolin	5316400	1
Henry Lamotte	Lanolin	5375500	2
Lamotte/Noweda	Lanolin	5375500	1
Henry Lamotte Oils GmbH...	Lanolin	5375500	2
lamotte	Lanolin	5447700	2
Lamotte/Anzag	Lanolin	5447700	1
Henry Lamotte/ Noweda	Lanolin	5517200	1
Henry/AHD	Lanolin	5651400	1
Lamotte/Alliance	Lanolin	5517200	1
HenryLamotte/Alliance	Lanolin	5517200	1
AHD	Lanolin	5517200	1
UNISAN	Lanolin	5651400	5
Sanacorp/ Henry Lamotte...	Lanolin	5651400	1
Lamotte	Lanolin	5651400	1
Henry Lamotte	Lanolin	5860800	1
Henry Lamotte Oils GmbH...	Lanolin	5860800	1
Lamotte GmbH	Lanolin	6000746001	1
Henry Lamotte Oils/AHD	Lanolin	6000746001	2
Bombastus	Lanolin	60080101	1
Bombastus	Lanolin	266981	1
Fargon	Lanolin	13b12-t01-001087	1
Sanacorp	Lanolin	14333602	1
Fargon	Lanolin	14k11-t01-016976	1
Caelo	Lanolin	16054702	1
Bombastus	Lanolin	294968	1
Caelo	Lanolin	2913U-01765	1
Caelo	Lanolin	1096249	1
Sanacorp	Lanolin	13062501	1
Sanacorp	Lanolin	13227601	2
Bombastus	Lanolin	282979	1
Bombastus	Lanolin	277968	1
Caelo	Lanolin	13326701-3455311103	1

- 57 491 spectra from 331 *Apo-Ident* customers from a total of 19 869 batches from a further 328 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 *Lanolin* 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 *Lanolin* 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	34 064
Type B	0	360	55	63 179
Type C	0	907	43	57 491

The substance/substance group *Lanolin* 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 % (> 99.9689 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9710 %)	86.7470 % (> 86.0241 %)
Type C	100.0000 % (> 99.5963 %)	95.4737 % (> 95.1579 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31003	32863	10.84	26.03
31439	31439	0.00	38.85
31746	31794	3.80	27.22
31794	31794	0.00	26.67
31795	31794	2.25	27.51
31798	31794	4.78	28.44
32863	32863	0.00	28.44

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Lauromacrogols
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30765-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lauromacrogols; Lauromacrogol 400; Macrogol 20 glycerol monostearate type II; Macrogol 20 glyceroli monostearas; Macrogol 4 lauryl ether; Macrogolglycerol hydroxystearate 40; Macrogolglyceroli - hydroxystearas; Macrogoli aether laurilicus; Macrogoli aether laurilicus 9; Polidocanolum; Polyethylenglycolum laurylicum; Polyoxyaethylenglycerinum monostearinicum; Polyoxyaethylenglycerinum trioxystearinicum; Polysorbate 20; Polysorbate 60; Polysorbatum 20; Polysorbatum 60

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Lauromacrogols*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Macrogolglycerol...	12L06-N02	30765	32	1405328
Caelo	Lauromacrogol 400	13095802	31025	40	20130523

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Polysorbate 60	12133619	31033	40	20120531
Fagron	Macrogol 20 glyc...	13H09-N06	31182	40	1407195
Caelo	Polysorbate 20	14019413	31323	40	AR-15-FG-008174-01
Caelo	Polysorbate 60	14027102	31324	40	AR-15-FG-008175-01
Caelo	Lauromacrogol 400	13340701	31372	40	AR-14-FG-012474-01
Caelo	Macrogol 4 laury...	14054401	31381	40	1507230
Caelo	Macrogol 20 glyc...	14033701	31469	40	20140214
Caelo	Macrogol 4 laury...	14225301	31583	40	20140820
Caelo	Macrogolglycerol...	14283805	31608	40	20141014
Caelo	Macrogolglycerol...	14283808	31625	40	AR-15-FG-010151-01
Fagron	Macrogolglycerol...	14283808	31640	40	20141208
Caelo	Polysorbate 20	14365105	31697	40	20150116
Euro OTC	Lauromacrogol 400	1510024	31768	40	20151102*
Euro OTC	Lauromacrogol 400	1605006	32283	40	20160531*
Fagron	Lauromacrogol 400	16E18-B04-326089	32824	40	20160527
Caelo	Polysorbate 60	170258	33058	40	20170313*
Caelo	Macrogol 4 laury...	16100205	33216	40	20160527

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 752 spectra of 19 reference samples from the substance/substance group *Lauromacrogols*. These samples are listed above in the [calibration samples](#) section.
- 33 592 spectra from a total of 780 batches from further 219 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 848 spectra of 25 reference samples from the substance/substance group *Lauromacrogols*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Polysorbate 20	81979119	30050	40
zu erfassen	Macrogol 4 lauryl ether	pending	30221	40
Caelo	Polysorbate 60	10037208	30230	40

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

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Supplier	Substance	Batch	Sample ID	Spectra
zu erfassen	Polysorbate 20	pending	30256	40
Caelo	Macrogol 4 lauryl ether	11014502	30278	40
Caelo	Polysorbate 20	1117205	30292	50
Fagron	Macrogolglycerol hydroxystea...	11C18-N08	30343	40
Fagron	Macrogol 20 glycerol monoste...	11E06-N07	30348	30
Caelo	Lauromacrogol 400	10228209	30364	30
zu erfassen	Macrogolglycerol hydroxystea...	pending	30503	40
Caelo	Macrogol 20 glycerol monoste...	10326003	30526	40
Caelo	Macrogol 4 lauryl ether	12057804	30530	40
Fagron	Lauromacrogol 400	12E03-N04	30573	40
Fagron	Lauromacrogol 400	12E03-N05	30594	40
Caelo	Macrogol 20 glycerol monoste...	14033701	31469 [†]	20
Caelo	Macrogol 4 lauryl ether	14225301	31583 [†]	20
Caelo	Macrogolglycerol hydroxystea...	14283805	31608 [†]	20
Caelo	Macrogolglycerol hydroxystea...	14283808	31625 [†]	20
Fagron	Macrogolglycerol hydroxystea...	14283808	31640 [†]	20
Caelo	Polysorbate 20	14365105	31697 [†]	20
Euro OTC	Lauromacrogol 400	1510024	31768 [†]	18
Caelo	Polysorbate 60	161771	32329	40
Caelo	Polysorbate 20	162335	32330	40
Caelo	Macrogol 20 glycerol monoste...	162800	32702	40
Euro OTC	Lauromacrogol 400	1610034	32816	40

- 62 746 spectra from a total of 1456 batches from further 434 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.

- 1654 spectra from 262 *Apo-Ident* customers from 417 batches from the substance/substance group *Lauromacrogols*.

Supplier	Substance	Batch	Spectra
Caelo	Macrogolglycerol hydroxystea...	13072004	10
Caelo	Macrogolglycerol hydroxystea...	14283808	4
Caelo	Macrogolglycerol hydroxystea...	14283813	7
Fagron	Macrogolglycerol hydroxystea...	14K28-B01	3
Fagron	Macrogolglycerol hydroxystea...	14K28B01301467	1
Fagron	Macrogolglycerol hydroxystea...	14K28-B01-301468	4
Caelo	Macrogolglycerol hydroxystea...	14k28-b01-301467	1
Caelo	Macrogolglycerol hydroxystea...	15169404	6
Caelo	Macrogolglycerol hydroxystea...	15169405	8
Calo/AHD	Macrogolglycerol hydroxystea...	16247401	1
Caelo	Macrogolglycerol hydroxystea...	16045403	5
Caelo	Macrogolglycerol hydroxystea...	12158602	2
Fagron	Macrogolglycerol hydroxystea...	16H05-B04-324748	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
Alliance H.	Macrogolglycerol hydroxystea...	15378302	1
Caelo	Macrogolglycerol hydroxystea...	12158606	10
Caelo	Macrogolglycerol hydroxystea...	2101415	1
Caelo	Macrogolglycerol hydroxystea...	12071402	1
Caelo	Macrogolglycerol hydroxystea...	16247401	1
Caelo	Macrogolglycerol hydroxystea...	13072008	3
Caelo	Macrogolglycerol hydroxystea...	13072005	1
Caelo	Macrogolglycerol hydroxystea...	14196805	10
Fagron	Macrogolglycerol hydroxystea...	14B14-B06-292160	7
Sanacorp	Macrogolglycerol hydroxystea...	14B14B06	1
Fagron	Macrogolglycerol hydroxystea...	14K28-801-301467	1
Fagron	Macrogolglycerol hydroxystea...	14B14-B06-295486	7
Fagron	Macrogolglycerol hydroxystea...	14B14-B06	4
Caelo	Macrogolglycerol hydroxystea...	29091402	1
BASF SE/ Phönix	Macrogolglycerol hydroxystea...	39658724U0	1
Caelo	Macrogolglycerol hydroxystea...	30091404	1
Fagron	Macrogolglycerol hydroxystea...	49426297V0	2
Caelo	Macrogolglycerol hydroxystea...	6021304	1
Caelo	Macrogolglycerol hydroxystea...	11161504	6
Caelo	Macrogolglycerol hydroxystea...	12103803	5
Phönix	Macrogolglycerol hydroxystea...	11161504	1
Kehr	Macrogolglycerol hydroxystea...	11K16-n09	1
Caelo	Macrogolglycerol hydroxystea...	12103807	5
Caelo	Macrogolglycerol hydroxystea...	1215614	1
Anzag 07.02.13 ek:4,70EUR	Macrogolglycerol hydroxystea...	12103807	1
Caesar & Loretz GmbH	Macrogolglycerol hydroxystea...	12158610	1
Caelo	Macrogolglycerol hydroxystea...	12158610	2
Caelo	Macrogolglycerol hydroxystea...	12158614	4
Caelo	Macrogolglycerol hydroxystea...	12158611	3
Fagron	Macrogolglycerol hydroxystea...	13D23-N03	13
Fagron	Macrogolglycerol hydroxystea...	12E11-N03	4
Fagron	Macrogolglycerol hydroxystea...	12L06-N02	12
Fagron	Macrogolglycerol hydroxystea...	13D23N03	3
Fagron	Macrogolglycerol hydroxystea...	13K07-N02	6
Großhandel	Macrogolglycerol hydroxystea...	13D23-N03	1
Caelo	Macrogolglycerol hydroxystea...	19111202	1
Sanacorp	Macrogolglycerol hydroxystea...	2/AKD16	1
Caelo	Macrogolglycerol hydroxystea...	21121203	1
Caelo	Macrogolglycerol hydroxystea...	17111202	1
Caelo	Macrogolglycerol hydroxystea...	26061303	1
Caelo	Macrogolglycerol hydroxystea...	20130912-1	1
Caelo	Macrogolglycerol hydroxystea...	26061304	1
Fagron	Macrogolglycerol hydroxystea...	87712168E0	1
Spinnrad	Macrogol 4 lauryl ether	12124000321	4
Noweda	Macrogol 4 lauryl ether	512400031	1
Gepepharm GmbH.	Lauromacrogol 400	130109	1
Caelo	Lauromacrogol 400	13095817	4
Caelo	Lauromacrogol 400	13340701	3
Großhandel	Lauromacrogol 400	13340703	1
Caelo	Lauromacrogol 400	13340703	3
Caelo	Lauromacrogol 400	13340710	2
Caelo	Lauromacrogol 400	13340706	1
Caelo	Lauromacrogol 400	13340712	1
Fagron	Lauromacrogol 400	13J01-N03	2
Caelo	Lauromacrogol 400	140911	5
Caelo	Lauromacrogol 400	14220805	1
Caelo	Lauromacrogol 400	14220806	1
Caelo	Lauromacrogol 400	14220808	1
Caelo	Lauromacrogol 400	14220813	3
Caelo	Lauromacrogol 400	14220816	4

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Supplier	Substance	Batch	Spectra
Fagron	Lauromacrogol 400	14H04-B03-301519	3
Caelo	Lauromacrogol 400	14220820	1
Caelo	Lauromacrogol 400	15192203	2
Caelo	Lauromacrogol 400	15192205	3
Caelo	Lauromacrogol 400	15192208	4
Caelo	Lauromacrogol 400	15192209	1
Caelo	Lauromacrogol 400	15363701	1
Caelo	Lauromacrogol 400	15363702	3
Caelo	Lauromacrogol 400	15363703	2
Caelo	Lauromacrogol 400	15363712	2
Caesar & Loretz/Sanacorp	Lauromacrogol 400	15363712	1
Devesa/NOW	Lauromacrogol 400	15363712	1
apomix PKH GmbH Halle	Lauromacrogol 400	15A26B02-30362	1
Caelo	Lauromacrogol 400	11107901	1
Caelo	Lauromacrogol 400	16102902	1
Fagron	Lauromacrogol 400	15A26-B02	4
Caelo	Lauromacrogol 400	12092512	3
Caelo	Lauromacrogol 400	12092501	2
Phönix Gotha	Lauromacrogol 400	12092516	1
Caelo	Lauromacrogol 400	12092525	3
Caelo	Lauromacrogol 400	12092516	4
Caelo	Lauromacrogol 400	12092530	2
Fagron	Lauromacrogol 400	12E03-N04	23
Fagron	Lauromacrogol 400	12A26-N08	9
gepepharm/Phoenix	Lauromacrogol 400	130109	4
GEHE	Lauromacrogol 400	130109	1
Caelo	Lauromacrogol 400	13095801	2
Caelo	Lauromacrogol 400	13095802	17
Sanacorp	Lauromacrogol 400	13095802	1
Caelo	Lauromacrogol 400	13095811	5
Caelo	Lauromacrogol 400	13095809	3
Anzag	Lauromacrogol 400	13A31N04	1
Fagron	Lauromacrogol 400	13A31-N04	3
Caelo	Macrogol 20 glycerol monoste...	13213601	1
Caelo	Macrogol 20 glycerol monoste...	14302001	1
Caelo	Macrogol 20 glycerol monoste...	13213602	3
Euro OTC	Macrogol 20 glycerol monoste...	15410502	1
Caelo	Macrogol 20 glycerol monoste...	15410502	1
Caelo	Macrogol 20 glycerol monoste...	14033701	2
Fagron	Macrogol 20 glycerol monoste...	12H23-N03	4
Caelo	Macrogol 20 glycerol monoste...	12326201	2
Fagron	Macrogol 20 glycerol monoste...	13H09-N06	5
Bombastus	Macrogol 20 glycerol monoste...	13H09-N06	1
Fagron	Macrogol 20 glycerol monoste...	ES61A85388	1
Caelo	Macrogol 20 glycerol monoste...	ES62A93607	1
Fagron	Macrogolglycerol hydroxystea...	13K07N02	3
phönix	Macrogolglycerol hydroxystea...	14196805	1
Sanacorp	Macrogolglycerol hydroxystea...	14196805	1
Sanacorp	Macrogolglycerol hydroxystea...	1423805	1
Caelo	Macrogolglycerol hydroxystea...	14283805	3
Alliance health	Macrogolglycerol hydroxystea...	14283808	1
Euro OTC	Macrogolglycerol hydroxystea...	1483808	1
Fagron	Macrogolglycerol hydroxystea...	14K28-B01-301467	8
Caelo	Macrogolglycerol hydroxystea...	14K28-B01-301467	1
AHD	Macrogolglycerol hydroxystea...	14B14-B06-295486	1
Fagron	Macrogolglycerol hydroxystea...	14B14-B06-2965486	1
Fagron	Macrogolglycerol hydroxystea...	14K28-B01-309197	2
Caelo	Macrogolglycerol hydroxystea...	14K28-B01-309197	1
Bombastus	Macrogolglycerol hydroxystea...	14K28-B01-309197	1
Caelo	Macrogol 4 lauryl ether	15041704	3

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Supplier	Substance	Batch	Spectra
Caelo	Macrogol 4 lauryl ether	15323701	6
Caelo	Macrogolglycerol hydroxystea...	15378302	6
Euro OTC	Macrogol 4 lauryl ether	15323704	1
Caelo	Macrogolglycerol hydroxystea...	15378304	1
Fagron	Macrogolglycerol hydroxystea...	15F18B10-309198	1
Caelo	Macrogolglycerol hydroxystea...	15378309	1
Fagron	Macrogolglycerol hydroxystea...	30378697V0	1
Caesar & Loretz GmbH Hi...	Macrogolglycerol hydroxystea...	16247401	1
Fagron	Macrogolglycerol hydroxystea...	11K16-N09	3
Caelo	Macrogolglycerol hydroxystea...	30378697V0	1
Fagron	Macrogolglycerol hydroxystea...	150056P0	1
Caelo	Macrogol 4 lauryl ether	4214A-02868	1
Fagron	Macrogolglycerol hydroxystea...	12D23-N03	1
Fagron	Macrogolglycerol hydroxystea...	12H24-N06	4
Noweda	Macrogolglycerol hydroxystea...	12H24-N06	1
Sanacorp	Macrogolglycerol hydroxystea...	13072004	1
Fagron	Macrogolglycerol hydroxystea...	13D23-N03	2
Fagron	Macrogolglycerol hydroxystea...	13G03-N18	4
Euro OTC	Macrogolglycerol hydroxystea...	28227168E0	1
Caelo	Macrogol 4 lauryl ether	7121201	1
Caelo	Macrogol 4 lauryl ether	12057804	4
Caelo	Macrogol 4 lauryl ether	12057806	4
Caelo	Macrogol 4 lauryl ether	12180202	3
Caelo	Macrogol 4 lauryl ether	12180204	3
Caelo	Macrogol 4 lauryl ether	13041706	3
Anzag	Macrogol 4 lauryl ether	12180204	1
Fagron	Macrogolglycerol hydroxystea...	11/26-N11	1
Caelo	Macrogolglycerol hydroxystea...	21071201	1
Fagron	Macrogolglycerol hydroxystea...	14B14-B06292160	2
Caelo	Macrogolglycerol hydroxystea...	14b14-b06-2921600855	1
Fagron	Macrogolglycerol hydroxystea...	14B14-B06-295468	1
Caelo	Macrogolglycerol hydroxystea...	14K28-B01-301468	1
Fagron	Macrogolglycerol hydroxystea...	15E18-B10	1
Fagron	Macrogolglycerol hydroxystea...	16H05-B04-326362	1
Fagron	Macrogolglycerol hydroxystea...	16H05-B04	1
Caelo	Macrogolglycerol hydroxystea...	4613M-01308	1
Fagron	Macrogolglycerol hydroxystea...	30378697Vo	1
Fagron	Macrogolglycerol hydroxystea...	509A372	1
Fafon/Anzag	Macrogolglycerol hydroxystea...	49426297V0	1
Post-Apotheke	Macrogolglycerol hydroxystea...	11K16-N09	1
Sanacorp	Macrogolglycerol hydroxystea...	12L06-N02	1
Fagron	Macrogolglycerol hydroxystea...	13d23-n03	1
Noweda	Macrogolglycerol hydroxystea...	13d23-N03	1
Phönix 31.01.2014	Macrogolglycerol hydroxystea...	13D23N03	1
Fargon	Macrogolglycerol hydroxystea...	13G03-N18	1
Gehe	Macrogolglycerol hydroxystea...	13K07-N02	1
Fagron	Macrogolglycerol hydroxystea...	8771216E0	1
Caelo	Macrogolglycerol hydroxystea...	13K07-N02	1
Phönix Gotha	Macrogolglycerol hydroxystea...	282268E0	1
Fagron	Macrogolglycerol hydroxystea...	87712168E0	1
Gehe	Macrogolglycerol hydroxystea...	11K16-N09	1
Caelo	Macrogolglycerol hydroxystea...	10236606	1
Noweda	Macrogolglycerol hydroxystea...	11C18-N08	1
Fagron	Macrogolglycerol hydroxystea...	79793775L0	1
gepepharm	Lauromacrogol 400	13-0108	2
Gehe	Macrogolglycerol hydroxystea...	79793775L0	1
Gepepharm	Lauromacrogol 400	130109	12
gebepfarm N PZN 01915345	Lauromacrogol 400	130109	1
gepepharm	Lauromacrogol 400	130109	29
gepepharm GmbH	Lauromacrogol 400	130109	17

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Supplier	Substance	Batch	Spectra
Fagron	Lauromacrogol 400	13K18-B30-288165	2
Fagron	Lauromacrogol 400	13K18-B30	3
Fagron	Lauromacrogol 400	14H04-B03	4
Fagron	Lauromacrogol 400	14H04-B03-297073	2
Fagron	Lauromacrogol 400	14E06-B05-293847	10
Fagron	Lauromacrogol 400	13F13-N07	3
Fagron	Lauromacrogol 400	13G02-N03	12
Löwen City-Apotheke Bar...	Lauromacrogol 400	2042015	1
GEHE	Macrogol 4 lauryl ether	21021172/5	1
Euro OTC	Lauromacrogol 400	1210035-01	2
Phönix	Lauromacrogol 400	13K18-B30-28816	2
Spinnrad	Macrogol 4 lauryl ether	1213400033	2
Euro OTC	Lauromacrogol 400	1306004-01	7
Fagron	Lauromacrogol 400	13-0599	2
Euro OTC	Lauromacrogol 400	1306004-02	3
Caelo	Macrogol 4 lauryl ether	13229805	6
Fagron	Lauromacrogol 400	13B13-N01	21
Fagron	Lauromacrogol 400	13G02N03	1
Fagron	Lauromacrogol 400	13g02-n03	1
Fagron	Lauromacrogol 400	13G02-N030021/1084	1
Fagron	Lauromacrogol 400	13G02-N030047/1084	1
Fagron	Lauromacrogol 400	13G02-N030515/1084	1
Caelo	Lauromacrogol 400	13K18-B30	1
Fagron	Lauromacrogol 400	13K18-B30288163	1
Fagron	Lauromacrogol 400	13K18-B30-288163	8
Caelo	Lauromacrogol 400	13K18-B30-288163	1
Fagron	Macrogol 4 lauryl ether	13K18-B30-288163	1
Fagron	Lauromacrogol 400	13K18-B30-288164	3
Caelo	Macrogol 4 lauryl ether	14054401	4
Euro OTC	Macrogol 4 lauryl ether	14054401	1
Euro OTC	Lauromacrogol 400	1407007-01	3
Euro OTC	Macrogol 4 lauryl ether	1407007-01	1
Fagron	Lauromacrogol 400	14-0731	3
Euro OTC	Lauromacrogol 400	1407007-07	1
Euro OTC	Lauromacrogol 400	1410010-01	1
Caelo	Lauromacrogol 400	1410010-10	1
Caelo	Macrogol 4 lauryl ether	14225306	2
Fagron	Macrogol 4 lauryl ether	14E06-B05-293846	1
Fagron	Lauromacrogol 400	14E06-B05-293846	2
Fagron	Lauromacrogol 400	14E06-B05-293848	3
Fagron	Lauromacrogol 400	14E06-B05-295979	2
Fagron	Lauromacrogol 400	14E06-B05293848	1
Fagron	Lauromacrogol 400	14E06-B05-29847	1
Euro OTC	Lauromacrogol 400	14H04-B03	2
GEHE 28.11.2014	Lauromacrogol 400	14H04-B03-297070	1
Fagron	Lauromacrogol 400	14H04-B03-297070	3
Caelo	Lauromacrogol 400	14H04-B03-297071	2
Fagron	Lauromacrogol 400	14H04-B03-297071	1
Fagron	Lauromacrogol 400	14H04-B03-297074	1
Fagron	Lauromacrogol 400	14H04-B03-301517	1
Euro OTC	Lauromacrogol 400	150303201	1
Euro OTC	Lauromacrogol 400	1503032-02	2
Euro OTC	Lauromacrogol 400	1510024-02	1
Fagron	Macrogol 4 lauryl ether	15A26B02	1
Euro OTC	Lauromacrogol 400	1503032-01	2
Schärer & Schläpfer AG/...	Lauromacrogol 400	15A26-02	1
Caelo	Lauromacrogol 400	1510024-02	1
Schärer & Schläpfer AG/...	Lauromacrogol 400	15A26-B02	1
Caelo	Macrogol 4 lauryl ether	15041801	2
Fagron	Lauromacrogol 400	15A26-B02-303625	6

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Supplier	Substance	Batch	Spectra
Euro OTC	Lauromacrogol 400	15A26-B02303628	1
Caelo	Lauromacrogol 400	15A26-B02-303627	1
Fagron	Lauromacrogol 400	15A26-B02-303626	1
Fagron	Lauromacrogol 400	15A26-B02-303627	1
Fagron	Lauromacrogol 400	15A26-B02-303628	7
Fagron	Lauromacrogol 400	15G10-B05	2
Fagron	Lauromacrogol 400	15G10-B05-314366	2
Fagron	Lauromacrogol 400	15G10-B05-31457	1
Caelo	Lauromacrogol 400	15G10-B05-313605	1
Fagron	Lauromacrogol 400	15G10-B05-315343	2
Fagron	Lauromacrogol 400	15G10-B05-31745	1
Fagron	Lauromacrogol 400	15G10-B05317456	2
Fagron	Lauromacrogol 400	15G10-B05-317457	2
Fagron	Lauromacrogol 400	15G10-B05-318670	1
Fagron	Lauromacrogol 400	15G1-B05-313605	1
Fagron	Lauromacrogol 400	16/149/P	1
Fagron	Lauromacrogol 400	16E18804-322722	1
Caelo	Lauromacrogol 400	16/077/M	1
Fagron	Lauromacrogol 400	16E18-804-321110	1
Fagron	Lauromacrogol 400	16E18-B04-322723	2
Fagron	Lauromacrogol 400	16E18-B04-324095	1
Caelo	Lauromacrogol 400	16E18-B04-322723	1
Fagron	Lauromacrogol 400	16E18-B04-321109	1
Caelo	Lauromacrogol 400	16E18-B04-327811	1
Euro OTC	Lauromacrogol 400	260315/1	1
Fagron	Lauromacrogol 400	9002-92-0	1
Fagron	Lauromacrogol 400	11I07-N05	1
Fagron	Lauromacrogol 400	12/18-N04	5
Fagron	Lauromacrogol 400	12-1074	1
Ebert+Jacobi	Lauromacrogol 400	12A26-N08	1
Fagron	Lauromacrogol 400	12e03-n04	1
Phönix	Lauromacrogol 400	12E03-N04	1
Fagron	Lauromacrogol 400	12I18-N04	2
gepepharm GmbH/Noweda	Lauromacrogol 400	130109	4
Fagron	Lauromacrogol 400	12I18-N04	1
Euro OTC	Lauromacrogol 400	1302014-01	4
EoRho	Lauromacrogol 400	1302014-01	2
Caelo	Lauromacrogol 400	1302014-01	2
Phönix Gotha	Lauromacrogol 400	13-0599	1
Fagron	Lauromacrogol 400	130599	1
Fagron	Lauromacrogol 400	13813-N01	3
Caelo	Lauromacrogol 400	13B13-N01	3
Noweda	Lauromacrogol 400	13B13-N01	1
Phönix Gotha	Lauromacrogol 400	13B13-N01	1
Schärer&Schläpfer AG/Ph...	Lauromacrogol 400	13B13-N01	1
Caesar/Noweda	Lauromacrogol 400	13B13-N01	1
Fagron	Lauromacrogol 400	13B13-No1	1
Fagron	Lauromacrogol 400	13B13-N01	1
Fagron	Lauromacrogol 400	13B-N01	1
Phönix Gotha	Lauromacrogol 400	13G02-N030461/1210	1
Fagron	Lauromacrogol 400	13G02-No3	2
Fargon	Lauromacrogol 400	13K18-B30-288166	1
Fagron	Lauromacrogol 400	13K18-B30-28816	1
Fagron	Lauromacrogol 400	21121201	1
Sanacorp	Lauromacrogol 400		1
Euro OTC	Lauromacrogol 400	221542	1
Euro OTC	Lauromacrogol 400	502956	1
Caelo	Lauromacrogol 400	3121505	1
Euro OTC	Lauromacrogol 400	1009020-02	2
Fagron	Lauromacrogol 400	11f28-n08	1

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Supplier	Substance	Batch	Spectra
Fagron	Lauromacrogol 400	11D28-N20	1
Caelo	Macrogol 4 lauryl ether	616A-02868	1
Caelo	Macrogol 4 lauryl ether	1014400032	3
Noweda 10.07.2015	Macrogol 4 lauryl ether	1014400032	1
Spinnrad	Macrogol 4 lauryl ether	1014400032	1
Sanacorp	Macrogol 4 lauryl ether	1014400032	1
Caelo	Macrogol 4 lauryl ether	14225303	3
Bombastus	Macrogol 4 lauryl ether	14225306	1
Caelo	Macrogol 4 lauryl ether	14225308	2
Caesar&loretz,Phoenix	Macrogol 4 lauryl ether	14225308	1
Hedinger	Macrogol 4 lauryl ether	15041704	1
Caesar & Loretz GmbH	Macrogol 4 lauryl ether	14225308	1
Caelo	Macrogol 4 lauryl ether	15323704	2
Spinnrad / Alliance HC	Macrogol 4 lauryl ether	314400031	1
Spinnrad/Sanacorp	Macrogol 4 lauryl ether	715400031	2
spinnrad	Macrogol 4 lauryl ether	715400031	2
Gehe/ Spinnrad	Macrogol 4 lauryl ether	715400031	1
Caelo	Macrogol 4 lauryl ether	1013400032	1
Spinnrad GmbH	Macrogol 4 lauryl ether	1013400032	1
Caesar & Loretz/Noweda	Macrogol 4 lauryl ether	715400031	1
Caelo	Macrogol 4 lauryl ether	3272779	1
Spinnrad	Macrogol 4 lauryl ether	101440032	1
spinnrad	Macrogol 4 lauryl ether	1213400033	1
Gehe	Macrogol 4 lauryl ether	1213400033	1
Noweda	Macrogol 4 lauryl ether	123400033	1
Spinnrad / Noweda	Macrogol 4 lauryl ether	1014400032	1
Caelo	Macrogol 4 lauryl ether	13229808	2
Caesar & Loretz	Macrogol 4 lauryl ether	14054401	1
Caelo	Macrogol 4 lauryl ether	14054405	4
Caesar & Loretz GmbH	Macrogol 4 lauryl ether	14054405	1
Raben-Apotheke Mildenau	Macrogol 4 lauryl ether	314400031	1
Caelo	Macrogol 4 lauryl ether	14225301	3
Caesar & Loretz GmbH Hi...	Macrogol 4 lauryl ether	14283001	1
Spinnrad GmbH / Phönix	Macrogol 4 lauryl ether	413400031	1
Spinnrad/Sanacorp	Macrogol 4 lauryl ether	314400031	2
Spinnrad GmbH	Macrogol 4 lauryl ether	314400031	1
Sanacorp	Macrogol 4 lauryl ether	1013400032	1
Spinnrad	Macrogol 4 lauryl ether	1111400032	2
Spinnrad GmbH	Macrogol 4 lauryl ether	1111400032	1
Noweda	Macrogol 4 lauryl ether	1111400032	1
Caesar & Loretz GmbH, 4...	Macrogol 4 lauryl ether	11220306	1
Gehe	Macrogol 4 lauryl ether	11220306	1
Spinnrad	Macrogol 4 lauryl ether	111140032	1
Caelo	Macrogol 4 lauryl ether	11220306	1
Spinnrad/Anzag	Macrogol 4 lauryl ether	12124000321	2
Gehe 12.04.2013	Macrogol 4 lauryl ether	12124000321	1
spinnrad	Macrogol 4 lauryl ether	1214000321	1
Gehe	Macrogol 4 lauryl ether	12180204	1
Caelo	Macrogol 4 lauryl ether	13041702	6
Caesar&loretz,Anzag	Macrogol 4 lauryl ether	13041702	1
AHD, 25.07.2013	Macrogol 4 lauryl ether	13136202	1
Caelo	Macrogol 4 lauryl ether	13136202	1
Jenne	Macrogol 4 lauryl ether	13136202	1
Caelo	Macrogol 4 lauryl ether	13229801	1
Gehe	Macrogol 4 lauryl ether	13136206	1
Spinnrad GmbH	Macrogol 4 lauryl ether	2240003	1
Caesar &Loretz GmbH	Macrogol 4 lauryl ether	13229802	1
Noweda	Macrogol 4 lauryl ether	413400031	2
Spinnrad	Macrogol 4 lauryl ether	413400031	4
Caelo	Macrogol 4 lauryl ether	20121112-1	1

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Supplier	Substance	Batch	Spectra
Spinnrad/Noweda	Macrogol 4 lauryl ether	413400031	1
Spinnrad/Phönix	Macrogol 4 lauryl ether	413400031	1
spinnrad	Macrogol 4 lauryl ether	512400031	1
Spinnrad / Noweda	Macrogol 4 lauryl ether	512400031	1
Spinnrad	Macrogol 4 lauryl ether	512400031	1
Spinnrad gmbh	Macrogol 4 lauryl ether	512400031	1
Caelo	Lauromacrogol 400	12345	1
Fagron	Lauromacrogol 400	130109	2
Fagron	Lauromacrogol 400	1314A-02384	1
Gepepharm/Phönix	Lauromacrogol 400	140911	2
gepepharm GmbH	Lauromacrogol 400	140911	3
gepepharm	Lauromacrogol 400	140911	13
gepepharm/Noweda	Lauromacrogol 400	140911	2
gegepharm	Lauromacrogol 400	140911	2
gepepharm GmbH / Allian...	Lauromacrogol 400	140911	1
gepepharm/Sanacorp	Lauromacrogol 400	14-1414	1
Caelo	Lauromacrogol 400	14H04-B03-301517	2
Euro OTC	Lauromacrogol 400	1510024-01	2
Croda Iberica	Lauromacrogol 400	1510024-02	1
Fagron	Lauromacrogol 400	15E27-B99-308668	1
Fagron	Lauromacrogol 400	15G10-B05-313605	1
Fagron	Lauromacrogol 400	15G10-B05-317456	2
Caelo	Lauromacrogol 400	15G10-B05-315343	1
Bombastus	Lauromacrogol 400	15G10-B05-318670	1
Fagron	Lauromacrogol 400	16-0290	1
gepepharm/Phoenix	Lauromacrogol 400	160312	2
Caelo	Lauromacrogol 400	16102903	1
Fagron	Lauromacrogol 400	16E18-B04-321110	2
Fagron	Lauromacrogol 400	16E18-B04-322722	1
GEPE/Anzag	Lauromacrogol 400	110408	2
Fagron	Lauromacrogol 400	T-190116-1	1
Gepepharm / Holdermann	Lauromacrogol 400	110408	8
Anzag	Lauromacrogol 400	110408	4
Caelo	Lauromacrogol 400	110408	14
Phoenix/gepepharm	Lauromacrogol 400	110408	1
Sanacorp	Lauromacrogol 400	110408	3
Gegepharm/N/26.02.13 PZ...	Lauromacrogol 400	110408	1
Fagron	Lauromacrogol 400	11F28-N08	2
Caesar & Lorenz	Lauromacrogol 400	13095802	1
Gehe	Lauromacrogol 400	130109	1
Sanacorp	Macrogol 4 lauryl ether	12180204	1
Fagron	Macrogol 4 lauryl ether	13B13N01	1
Gutenberg-Apotheke	Macrogolglycerol hydroxystea...	13072008	1
Hedinger	Macrogolglycerol hydroxystea...	13333702	1
Fagron	Macrogolglycerol hydroxystea...	153356P0	1
Caelo	Macrogolglycerol hydroxystea...	P146/14	1
Caelo	Polysorbate 20	714E-02525	1
	Macrogolglycerol hydroxystea...	13D23-N03	1
Caelo	Polysorbate 20	1709930	1
Caelo	Polysorbate 20	12031605	1
Caelo	Polysorbate 20	13086509	10
Phoenix	Polysorbate 20	13086517	1
Caelo	Polysorbate 20	13086517	11
Caelo	Polysorbate 60	13258902	3
Caelo	Polysorbate 20	13297005	11
Euro OTC	Polysorbate 20	13297009	1
gehe	Polysorbate 20	13297009	1
Caelo	Polysorbate 20	13297009	6
Caelo	Polysorbate 20	13297010	17
gehe	Polysorbate 20	13297099	1

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Supplier	Substance	Batch	Spectra
Fagron	Polysorbate 20	13J18-B02-287378	3
Fagron	Polysorbate 20	13J18-B02	1
Caelo	Polysorbate 20	14019410	5
Phönix	Polysorbate 20	14019410	1
Caelo	Polysorbate 20	14019418	15
Cealo	Polysorbate 20	14019418	1
Gehe	Polysorbate 60	14027102	1
Caelo	Polysorbate 60	14027103	1
Caelo	Polysorbate 20	14041503	1
Caelo	Polysorbate 20	14213213	6
Caelo	Polysorbate 20	14365105	11
Caelo	Polysorbate 20	14213211	2
Euro OTC	Polysorbate 20	14213213	1
Caelo	Polysorbate 20	14365109	14
Caelo	Polysorbate 20	14365116	17
Phönix	Polysorbate 20	14365116	2
Fagron	Polysorbate 20	14A23-B01	1
Caelo	Polysorbate 60	15067401	2
Caelo	Polysorbate 60	15067407	1
Caesar&Loretz GmbH	Polysorbate 60	15067409	1
Caelo	Polysorbate 20	15159004	1
Caelo	Polysorbate 20	1532302	1
Noweda	Polysorbate 20	15323902	1
Caelo	Polysorbate 20	15323902	7
Caelo	Polysorbate 20	15323912	5
Caesar & Loretz GmbH Hi...	Polysorbate 20	15323902	1
Caelo	Polysorbate 20	1532902	1
Caelo	Polysorbate 60	16007302	1
Caelo	Polysorbate 20	16029703	17
Caelo	Polysorbate 20	16114502	2
Caelo	Polysorbate 20	16114503	5
Caelo	Polysorbate 20	16233501	3
Caelo	Polysorbate 20	3114I-02525	1
Caelo	Polysorbate 20	1912M-02525	1
Caelo	Polysorbate 20	611poly	1
Caelo	Polysorbate 20	11117201	1
Caelo	Polysorbate 20	11117205	2
Caelo	Polysorbate 20	11179506	2
Caelo	Polysorbate 20	11179511	5
Noweda	Polysorbate 20	11347701	1
Phönix Gotha	Polysorbate 20	11347701	1
Caelo	Polysorbate 20	11347702	1
Caelo	Polysorbate 20	11347707	6
Phönix	Polysorbate 20	11347707	1
VDL	Polysorbate 20	11347707	1
Caelo	Polysorbate 20	11347711	8
Sanacorp	Polysorbate 20	11347711	1
Caelo	Polysorbate 20	11347715	7
Caelo	Polysorbate 20	11347719	10
Caelo	Polysorbate 20	12303006	7
Fagron	Polysorbate 20	11I15-N13	1
Noweda	Polysorbate 20	12303016	1
Anzag	Polysorbate 20	12303006Caelo	1
Caelo	Polysorbate 20	12303016	14
Sanacorp	Polysorbate 20	12345	1
Caelo	Polysorbate 20	13066512	1
GEHE	Polysorbate 20	13086505	1
Caelo	Polysorbate 20	13086505	2
Sanacorp	Polysorbate 20	13086509	2
Caelo	Polysorbate 20	13086510	1

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Supplier	Substance	Batch	Spectra
Caelo	Polysorbate 20	13086512	15
Sanacorp	Polysorbate 20	13086517	1
Alliance Health 15.10.2...	Polysorbate 20	13086517	1
Caelo	Polysorbate 20	1329001	1
Caelo	Polysorbate 20	13297001	8
Bombastus	Polysorbate 20	13297001	1
Phönix Gotha	Polysorbate 20	13297005	1
Caelo	Polysorbate 20	20210312-1	1
Caelo	Polysorbate 20	2704212525	1
Caelo	Polysorbate 20	19021303	1
Caelo	Polysorbate 20	20220312-1	1
Caelo	Polysorbate 20	2713E2525	1
Caelo	Polysorbate 20	80479168	1
Caelo	Polysorbate 20	4612A-02525	1
Caelo	Polysorbate 20		1
Caelo	Polysorbate 60	12133602	1
Caelo	Polysorbate 60	13098006	1
Caelo	Polysorbate 60	12133611	2
Caelo	Polysorbate 60	12133612	1
Gehe am 06.02.2014	Polysorbate 60	13258902	1
Caelo	Polysorbate 20	11347701	1
Sanacorp	Polysorbate 20	12303006	1
Caelo	Polysorbate 20	13297001-3449311132	1
Caelo	Macrogol 20 glycerol monoste...	3042223	1
gepepharm GmbH	Lauromacrogol 400	1915345	1
Gepepharm über Phoenix	Lauromacrogol 400	130109	7
gepepharm/Otto	Lauromacrogol 400	130109	25
gepepharm/AHD	Lauromacrogol 400	130109	1
gepepharm/Sanacorp	Lauromacrogol 400	130109	7
gepepharm /Noweda	Lauromacrogol 400	130109	3
Gepepharm / Noweda	Lauromacrogol 400	140911	1
Phoenix	Lauromacrogol 400	140911	1
Gepepharm über Phoenix	Lauromacrogol 400	140911	3
gepepharm GmbH/ NOW	Lauromacrogol 400	140911	1
gepepharm/Phönix	Lauromacrogol 400	140911	4
Gepepharm/Sanacorp	Lauromacrogol 400	140911	9
Gepepharm	Lauromacrogol 400	140911	3
Noweda/gepepharm	Lauromacrogol 400	140911	1
Gepepharm/Noweda	Lauromacrogol 400	140911	3
gepepharm/Gehe	Lauromacrogol 400	140911	3
Phönix Gotha	Lauromacrogol 400	140911	1
gepep/Phoenix	Lauromacrogol 400	140911	1
phoenix/noveda	Lauromacrogol 400	140911	2
gepepharm / Phönix	Lauromacrogol 400	140911	2
Fiebig/ gepepharm	Lauromacrogol 400	140911	1
Hedinger/ Sanacorp	Lauromacrogol 400	140911	1
Gepepharm GmbH	Lauromacrogol 400	140911	1
gepepharm / Noweda	Lauromacrogol 400	140911	1
Kehr/gepepharm	Lauromacrogol 400	140911	1
Gepepharm/Sana	Lauromacrogol 400	140911	1
Ebert & Jacobi 31.05...	Lauromacrogol 400	140911	2
Audor Pharma	Lauromacrogol 400	140911	2
Caelo	Lauromacrogol 400	14-1414	1
Gepepharm/ Gehe	Lauromacrogol 400	14-1414	1
Caelo	Lauromacrogol 400	15363707	1
Fagron	Lauromacrogol 400	15A26B02-303627	1
Fagron	Lauromacrogol 400	15C10-B05-314366	1
Sanacorp	Lauromacrogol 400	160290	1
Caelo	Lauromacrogol 400	160312	1
gepepharm GmbH/Kehr	Lauromacrogol 400	160312	1

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Supplier	Substance	Batch	Spectra
Caelo	Lauromacrogol 400		1
Gepepharm/Alliance	Lauromacrogol 400	160312	1
Fagron	Lauromacrogol 400	2215I-02384	1
gebepharma	Lauromacrogol 400	813E-02384	1
Gepepharm	Lauromacrogol 400	6111203	1
Gepepharm/Kehr	Lauromacrogol 400	51123/2Sie	1
gebepharma	Lauromacrogol 400	813Q-02384	1
Hersteller: gepepharm G...	Lauromacrogol 400	90807	1
Caelo	Lauromacrogol 400	90807	1
gepepharm/Phönix	Lauromacrogol 400	1101409	1
Gepepharm	Lauromacrogol 400	110408	6
Ichthyol	Lauromacrogol 400	110408	4
Gepepharm / Gehe	Lauromacrogol 400	110408	1
Gepepharm GmbH	Lauromacrogol 400	110408	4
Gehe	Lauromacrogol 400	110408	6
gepepharm	Lauromacrogol 400	110408	2
gepepharm GmbH	Lauromacrogol 400	110408	7
Noweda	Lauromacrogol 400	110408	4
Phoenix	Lauromacrogol 400	110408	1
Gepepharm/VDL	Lauromacrogol 400	110408	3
Gepepharm/Gehe	Lauromacrogol 400	110408	2
Gepepharm Anzag	Lauromacrogol 400	110408	13
Kehr	Lauromacrogol 400	110408	1
gepepharm,Anzag	Lauromacrogol 400	110408	2
Gepepharm / Sanacorp	Lauromacrogol 400	110408	2
Phönix/Gepepharma	Lauromacrogol 400	110408	6
gepepharm	Lauromacrogol 400	110408	5
ANZAG	Lauromacrogol 400	110408	2
gepepharm, Noweda	Lauromacrogol 400	110408	4
gepepharm/Phönix	Lauromacrogol 400	110408	2
Stumpf/gepepharm	Lauromacrogol 400	110408	1
Phoenix (gepepharm)	Lauromacrogol 400	110408	1
gepepharm/gehe	Lauromacrogol 400	110408	3
Gehe 12.04.2013	Lauromacrogol 400	110408	1
Gebepharma/Anzag	Lauromacrogol 400	110408	1
Geopharm	Lauromacrogol 400	110408	1
gepepharmGmbH	Lauromacrogol 400	110408	1
Gepepharm GmbH / Anzag	Lauromacrogol 400	110408	1
gepepharm / Noweda	Lauromacrogol 400	110408	1
Euro OTC	Lauromacrogol 400	1109011-01	2
Caelo	Lauromacrogol 400	11107905	1
Caelo	Lauromacrogol 400	11107804	1
Caelo	Lauromacrogol 400	11107906	1
Caelo	Lauromacrogol 400	12092509	1
Fagron	Lauromacrogol 400	12-0719	1
Fagron	Lauromacrogol 400	12A26-N08	1
Fagron	Lauromacrogol 400	1218n04	1
Caelo	Lauromacrogol 400	12A26-N08	1
Caelo	Lauromacrogol 400	12E03-N04	1
gepepharm GmbH	Lauromacrogol 400	13-0108	1
Sanacorp	Lauromacrogol 400	130108	1
gepepharm / Sanacorp	Lauromacrogol 400	13-0108	1
Phönix	Lauromacrogol 400	13-0108130109	1
gepepharm/Phönix	Lauromacrogol 400	130109	5
Gebepharma/Anzag	Lauromacrogol 400	130109	1
Phoenix	Lauromacrogol 400	13-0108	1
gepepharm/Noweda	Lauromacrogol 400	130109	2
gepepharm GmbH/ Noweda	Lauromacrogol 400	130109	1
Gepepharm / Gehe	Lauromacrogol 400	130109	6
gepepharm / Sanacorp	Lauromacrogol 400	130109	6

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Supplier	Substance	Batch	Spectra
Gegepharm/Gehe	Lauromacrogol 400	130109	5
Phönix/Gepepharma	Lauromacrogol 400	130109	4
Caelo	Lauromacrogol 400	130109	8
gepepharm GmbH	Lauromacrogol 400	13-0109	1
gepepharm GmbH	Lauromacrogol 400	130109	1
gepepharm/sanacorp	Lauromacrogol 400	130109	1
Gepepharm/Noweda	Lauromacrogol 400	130109	12
Gegepharm	Lauromacrogol 400	130109	2
Phönix/gepepharm	Lauromacrogol 400	130109	3
gepepharm/ Noweda	Lauromacrogol 400	130109	6
Sanacorp	Lauromacrogol 400	130109	1
Gepepharm/Phönix	Lauromacrogol 400	130109	5
gepepharm, Noweda	Lauromacrogol 400	130109	1
gegepharm	Lauromacrogol 400	130109	1
Gepegepharm	Lauromacrogol 400	130109	1
Gepepharm GmbH / Anzag	Lauromacrogol 400	130109	1
gepe/Gehe	Lauromacrogol 400	130109	1
gepepharm/Phönix	Lauromacrogol 400	130109	1
Phönix Gotha	Lauromacrogol 400	130109	3
gehe	Lauromacrogol 400	130109	2
Gepepharm/V.d.L.	Lauromacrogol 400	130109	1
Gepepharm/Phoenix	Lauromacrogol 400	130109	2
Gepepharm/ Noweda	Lauromacrogol 400	130109	1
gepepharm / Noweda	Lauromacrogol 400	130109	5
Phoenix	Lauromacrogol 400	130109	1
Gepepharm/Sanacorp	Lauromacrogol 400	130109	1
gepepharm/Gehe	Lauromacrogol 400	130109	3
gepepharm GmbH / Allian. ...	Lauromacrogol 400	130109	1
gepepharm gmbh	Lauromacrogol 400	130109	2
Gepepharm / GEHE	Lauromacrogol 400	130109	1
Noweda/gepepharm	Lauromacrogol 400	130109	1
gepepharm/Kehr	Lauromacrogol 400	130199	1
gepepharm	Lauromacrogol 400	13044009	1
Caelo	Lauromacrogol 400	13-0599	1
Gepepharm	Lauromacrogol 400	13051502	1
Fagron	Lauromacrogol 400	13-1827	1
Phönix	Lauromacrogol 400	13B13-N01	1
GEHE	Lauromacrogol 400	13B13-N01	1
Euro OTC	Lauromacrogol 400	13F13-N07	1
Hedinger/Gehe	Lauromacrogol 400	13G02-N03	1
Großhandel	Lauromacrogol 400	13J01-N03	1
Calo/AHD	Lauromacrogol 400	14-0731	1
GEPEPHARM	Lauromacrogol 400	140911	5
Gepepharm GmbH	Lauromacrogol 400	140911	5
Phoenix/gepepharm	Lauromacrogol 400	140911	3
Fagron	Lauromacrogol 400	14H04B03	1
Gepepharm	Lauromacrogol 400	17111403	1
GEPEPHARM	Lauromacrogol 400	14-1414	1
Caelo	Lauromacrogol 400	14220807	1
Gepepharm/Phoenix	Lauromacrogol 400	1614U2384	1
Gepepharm	Lauromacrogol 400	2002312384	1
Gepepharm	Lauromacrogol 400	19101201	1
gebepharma	Lauromacrogol 400	20030412-1	1
Gepepharm	Lauromacrogol 400	19121203	1
Caelo	Lauromacrogol 400	21011501	1
Gepepharm	Lauromacrogol 400	25061502	1
Gepepharm	Lauromacrogol 400	27111202	1
Gepepharm/Phoenix	Lauromacrogol 400	3813E02384	1
Gepepharm	Lauromacrogol 400	30031303	1
Gepepharm	Lauromacrogol 400	4111M-02384	1

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Supplier	Substance	Batch	Spectra
Fagron	Lauromacrogol 400	3713U-02384	1
gepepharm/Otto	Lauromacrogol 400	65793	1
Phönix Gotha	Polysorbate 20	14365116	1
Caelo	Polysorbate 20	2215I-02525	1
Caelo	Polysorbate 20	3478	1
Berkel AHK	Polysorbate 20	14019418	1
Fagron	Polysorbate 20	14A23-B01-294167	1
Caelo	Polysorbate 20	2112E-02525	1
Sanacorp	Polysorbate 20	4/AKD1	1

- 56 787 spectra from 332 *Apo-Ident* customers from a total of 19 681 batches from a further 323 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 *Lauromacrogols* 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 *Lauromacrogols* 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	752	0	33 592
Type B	0	816	32	62 746
Type C	0	1577	77	56 787

The substance/substance group *Lauromacrogols* 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 % (> 99.9689 %)	100.0000 % (> 99.2021 %)
Type B	100.0000 % (> 99.9710 %)	96.2264 % (> 95.8726 %)
Type C	100.0000 % (> 99.5963 %)	95.3446 % (> 95.1632 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30765	30765	0.00	22.20
31025	32283	2.00	23.97
31033	31324	5.38	21.91
31182	31182	0.00	18.38
31323	31323	0.00	24.06
31324	31324	0.00	18.05
31372	31372	0.00	26.72
31381	31381	0.00	23.09
31469	31182	4.64	21.11
31583	31381	7.40	20.95
31608	30765	12.14	26.26
31625	31625	0.00	28.66
31640	31625	4.76	26.97
31697	31323	10.34	24.48
31768	31768	0.00	26.96
32283	32283	0.00	25.69
32824	31324	12.93	38.89
33058	33058	0.00	22.82
33216	31381	8.27	25.59

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Lavender oil / Clary sage oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30861-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Lavender oil / Clary sage oil; Clary sage oil; Lavandulae aetheroleum; Lavender oil; Oleum lavandulae artificiale; Oleum salviae sclarea

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Lavender oil / Clary sage oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lavender oil	12201206	30861	40	20120721
Fagron	Lavender oil	13D24-N01	31223	40	AR-15-FG-009308-01
Caelo	Lavender oil	12201213	31237	30	20120721

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lavender oil	12334514	31238	30	20121120
Caelo	Clary sage oil	13334802	31413	40	1509218
Caelo	Lavender oil	13252605	31416	40	20130802
Caelo	Lavender oil	13252207	31422	40	20130802
Euro OTC	Lavender oil	1312008-01	31528	40	AR-15-FG-000438-01
Caelo	Clary sage oil	1431102	31668	40	20141031
Euro OTC	Lavender oil	1507031	31721	40	0000010673
Euro OTC	Lavender oil	1510040	31800	40	20151119*
Euro OTC	Lavender oil	1608026	32710	40	20160902*
Fagron	Lavender oil	15I03-B01-314158	32996	40	20150916

Validation samples

A total of 156379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 500 spectra of 13 reference samples from the substance/substance group *Lavender oil / Clary sage oil*. These samples are listed above in the [calibration samples](#) section.
- 33844 spectra from a total of 785 batches from further 223 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 300 spectra of 10 reference samples from the substance/substance group *Lavender oil / Clary sage oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lavender oil	13252207	31422 [†]	20
Euro OTC	Lavender oil	1312008-01	31528 [†]	20
Caelo	Clary sage oil	1431102	31668 [†]	20
Euro OTC	Lavender oil	1507031	31721 [†]	20
Euro OTC	Lavender oil	1510040	31800 [†]	20
Euro OTC	Lavender oil	1601053	31997	40
Euro OTC	Lavender oil	1606004	32458	40
Caelo	Lavender oil	162922	32684	40
Euro OTC	Lavender oil	1610029	32834	40
Euro OTC	Lavender oil	1701005	32986	40

*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.

- 63 294 spectra from a total of 1467 batches from further 438 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.

- 544 spectra from 156 *Apo-Ident* customers from 206 batches from the substance/substance group *Lavender oil / Clary sage oil*.

Supplier	Substance	Batch	Spectra
Fagron	Lavender oil	13B22-N02	12
Caelo	Lavender oil	13252603	1
Fagron	Lavender oil	14D14-B02	3
Caelo	Lavender oil	15043504	6
Caelo	Lavender oil	13252621	1
Caelo	Lavender oil	15278102	2
Caelo	Lavender oil	15043516	1
Fagron	Lavender oil	12B16-N02	4
Caelo	Lavender oil	273289	1
Taoasis	Lavender oil	LOG2014-119488	2
Caelo	Lavender oil	7111403	1
Taoasis	Lavender oil	LOG2014-121513	2
Taoasis	Lavender oil	LOG2014-120278	1
Caelo	Lavender oil	12334513	10
Fagron	Lavender oil	11K2900-0002	1
Fagron	Lavender oil	12H15-N01	11
Fagron	Lavender oil	13/11-B03-289423	1
Taoasis	Lavender oil	130201-115678	1
Taoasis / Sanacorp	Lavender oil	130201-115678	1
Taoasis	Lavender oil	130201-116395	2
Taoasis	Lavender oil	130201-116899	6
Caelo	Lavender oil	13133703	9
PHOENIX 05.05.2014	Lavender oil	130202301	1
Noweda	Lavender oil	13133703	2
GEHE 17.05.2014	Lavender oil	13133703	1
Caelo	Lavender oil	13133705	1
Caelo	Lavender oil	13133704	3
Caelo	Lavender oil	13133706	19
Caelo	Lavender oil	13133715	11
Caelo	Lavender oil	13252201	5
Caelo	Lavender oil	13202218	1
Noweda	Lavender oil	13252201	1
Caelo	Lavender oil	13252202	5
Caelo	Lavender oil	13252204	6
Caelo	Lavender oil	13252206	3
Caelo	Lavender oil	13252207	4
Caelo	Lavender oil	13252220	6
Caelo	Lavender oil	13252218	1
Phönix	Lavender oil	13252220	2

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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
Caelo	Lavender oil	13252225	4
Caelo	Lavender oil	13252616	2
Caelo	Lavender oil	13252611	1
Fagron	Lavender oil	13D24N01	3
Fagron	Lavender oil	13D24-N01	4
Fagron	Lavender oil	13E30-B01	4
Fagron	Lavender oil	13E30-B01-285544	4
Fagron	Lavender oil	13E30-B01-285543	1
Fagron	Lavender oil	13e30-b01-285544	1
Fagron	Lavender oil	13J11B03	1
Fagron	Lavender oil	13G11-N04	10
Fagron	Lavender oil	13G11N04	1
Caelo	Lavender oil	13E30-B01-285545	1
Sanacorp	Lavender oil	13G11-N04	1
Fagron	Lavender oil	13J11-B03	4
Fagron	Lavender oil	13J11-B03-289423	4
Fagron	Lavender oil	13J11-B03-289424	1
Caelo	Lavender oil	13J11-B03-289424	1
Fagron	Lavender oil	13J11-B03-289425	1
Caelo	Lavender oil	1414-B02-302035	1
Fagron	Lavender oil	13J11-BC3-289423	1
Caelo	Lavender oil	1421831	1
Caelo	Lavender oil	14218311	9
Caelo	Lavender oil	14218301	1
Caelo	Lavender oil	14218314	5
Caelo	Lavender oil	14218312	1
Caelo	Lavender oil	14218322	5
Caelo	Lavender oil	14218321	1
Frey & Lau GmbH/Phoenix	Lavender oil	14A07-B02-289955	1
Fagron	Lavender oil	14A07-B02-289955	1
Fagron	Lavender oil	14A07-B02	2
Fagron	Lavender oil	14A07B02	1
Caelo	Lavender oil	14218324	1
Fagron	Lavender oil	14A07-B02-294931	4
Caelo	Lavender oil	14A07-B02-289955	1
Fagron	Lavender oil	14D14B02	1
Fagron	Lavender oil	14D14-B02-302034	2
Fagron	Lavender oil	15/03-B01-314158	1
Euro OTC	Lavender oil	1503006-01	2
Caelo	Lavender oil	15043505	1
Caelo	Lavender oil	15043512	1
Caelo	Lavender oil	15043518	3
Caelo	Lavender oil	15043525	8
Caelo	Lavender oil	15043520	1
Euro OTC	Lavender oil	15043525	2
Caelo	Lavender oil	15043526	4
Euro OTC	Lavender oil	1507031-01	1
Caelo	Lavender oil	1510040-01	2
Caelo	Lavender oil	15363302	11
AHD	Lavender oil	15363302	1
Caelo	Lavender oil	15363310	3
Fagron	Lavender oil	15B10-B07-304078	1
Euro OTC	Lavender oil	15B10-B07	1
Caelo	Lavender oil	15363304	4
Fagron	Lavender oil	15C26-B02-310775	1
Caelo	Lavender oil	17041502	1
Caelo	Lavender oil	17051404	1
Caelo	Lavender oil	2189	1
Taoasis	Lavender oil	22015-122102	1
Bombastus	Lavender oil	275898	1

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Supplier	Substance	Batch	Spectra
Bombastus	Lavender oil	279919	5
Bombastus	Lavender oil	284486	1
Bombastus	Lavender oil	287254	3
Noweda	Lavender oil	284691	1
Bombastus	Lavender oil	288979	3
Bombastus	Lavender oil	293661	3
Noweda	Lavender oil	293661	1
Bombastus	Lavender oil	295738	2
InfectoPharm/Noweda	Lavender oil	297733	1
Bombastus	Lavender oil	297733	2
Caelo	Lavender oil	31031501	1
Taoasis	Lavender oil	43703-122404	1
Taoasis/Taoasis	Lavender oil	30560-112844	1
Taoasis	Lavender oil	4651010-118091	1
Taoasis	Lavender oil	4651010118091	1
Caelo	Lavender oil	480435519	1
Fagron	Lavender oil	736340	1
Fagron	Lavender oil	759243	1
phönix	Lavender oil	759243	1
Caelo	Lavender oil	1021403	1
Caelo	Lavender oil	780162	1
Caelo	Lavender oil	3011401	1
Fagron	Lavender oil	794323	1
Caelo	Lavender oil	213A-01990	1
Fagron	Lavender oil	612211990	2
Caelo	Lavender oil	3091207	1
Fagron	Lavender oil	780162	1
Caelo	Lavender oil	11053709	5
Caelo	Lavender oil	11221308	1
Noweda	Lavender oil	11221315	2
Noweda	Lavender oil	11221309	1
Caesar & Loretz GmbH, 4...	Lavender oil	11355	1
Caelo	Lavender oil	11221315	1
Fagron	Lavender oil	11F09-N07	1
Fagron	Lavender oil	11K17-N06	2
Fagron	Lavender oil	11L22-N16	4
Phönix	Lavender oil	11L22-N16	1
Caelo	Lavender oil	12056802	4
Caesar & Loretz GmbH, 4...	Lavender oil	12056804	1
Caelo	Lavender oil	12056804	2
Caelo	Lavender oil	12056807	1
Caelo	Lavender oil	12056809	16
gehe.01.2013	Lavender oil	12056809	1
Caelo	Lavender oil	12056814	5
Phönix, 16.10.2012	Lavender oil	12056814	1
Caelo	Lavender oil	12056815	1
Noweda	Lavender oil	12056815	1
Caelo	Lavender oil	12056820	1
Caelo	Lavender oil	12056816	3
Caelo	Lavender oil	12056821	2
Caesar & Loretz/ Noweda	Lavender oil	12056816	1
Sanacorp	Lavender oil	12056821	1
Noweda	Lavender oil	12056821	1
Caelo	Lavender oil	12056822	11
Caelo	Lavender oil	12201201	1
Caelo	Lavender oil	12081301	2
Caelo	Lavender oil	12201213	2
Caelo	Lavender oil	12201206	1
Caelo	Lavender oil	12201215	1
Caelo	Lavender oil	123344514	1

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Supplier	Substance	Batch	Spectra
Caelo	Lavender oil	12334501	6
Caelo	Lavender oil	12334503	2
Caelo	Lavender oil	12334507	4
Großhandel	Lavender oil	12334507	1
Caelo	Lavender oil	12334510	7
Caesar & Loretz GmbH D-...	Lavender oil	12334510	2
Anzag 10.04.13 ek: 5.83EUR	Lavender oil	12334510	1
Sanacorp	Lavender oil	12334513	1
Caelo	Lavender oil	12334514	5
Fagron	Lavender oil	12334516	2
Caelo	Lavender oil	12334516	5
geile	Lavender oil	12334516	1
Caelo	Lavender oil	1234501	1
AHC 22.08.13 EK5,83 25ml	Lavender oil	12334516	1
Caelo	Lavender oil	123456	1
Caelo	Lavender oil	1234514	2
Caelo	Lavender oil	1245	1
Fagron	Lavender oil	12D05-N02	6
Phönix	Lavender oil	12D05-N02	1
Caelo	Lavender oil	12H15-N01	3
Taoasis	Lavender oil	130201-115396	1
Caelo	Lavender oil	12H15-No1	1
Gehe	Lavender oil	12H15-N01	1
Fagron	Lavender oil	13097R	1
Caelo	Lavender oil	13071302	1
Euro OTC	Lavender oil	1302023-01	1
Caesar & Loretz GmbH, 4...	Lavender oil	13133706	1
Gehe	Lavender oil	13252601	1
Fagron	Lavender oil	13B22N02	2
Caelo	Lavender oil	13B22-No2	1
Fagron	Lavender oil	13B22-N02	1
Fagron	Lavender oil	13D24-N01	1
AHD, 25.11.13	Lavender oil	13G11-N04	1
PVL	Lavender oil	1401110	1
primavera	Lavender oil	1480513	1
Caelo	Lavender oil	15081301	1
Euro OTC	Lavender oil	15100-40-01	1
Euro OTC	Lavender oil	1510040-01	1
Caelo	Lavender oil	15278101	1
Caelo	Lavender oil	15363004	1
Caelo	Lavender oil	15363303	1
Fagron	Lavender oil	15B10-B07-304079	1
Fagron	Lavender oil	15C26-B02-314159	1
Caelo	Lavender oil	16023003	1
Fagron	Lavender oil	1601311990	1
Caelo	Lavender oil	16101203	1
Fagron	Lavender oil	16A07-B01-32195	1
Jenne	Lavender oil	192900-0003	1
Taoasis	Lavender oil	22015-122995	2
Phönix, 23.10.2012	Lavender oil	271465	1
Bombastus	Lavender oil	272797	5
Fiebi 29.09.12 ek:8,95	Lavender oil	271465	1
Anzag 15.11.2012	Lavender oil	270560	1
Hedinger	Lavender oil	273007	1
Bombastus	Lavender oil	273725	1
Bombastus	Lavender oil	273007	1
Bombastus	Lavender oil	273980	2
Anzag 10.04.13 ek: 9,57EUR	Lavender oil	273725	1
Caelo	Lavender oil	276783	1
Bombastus	Lavender oil	276783	2

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Supplier	Substance	Batch	Spectra
Bombastus	Lavender oil	300666	2
Caelo	Lavender oil	30081301	1
Taoasis	Lavender oil	30560-110088	1
Taoasis GmbH	Lavender oil	30560	1
Taoasis	Lavender oil	30560-108326	1
Taoasis	Lavender oil	30560-111623	2
Taoasis	Lavender oil	30560-113019	1
Fagron	Lavender oil	5013I1990	1
Caelo	Lavender oil	4110E-01990	1
Taoasis	Lavender oil	30560-113018	1
Noweda	Lavender oil		1
Caelo	Lavender oil	559621	1
Fagron	Lavender oil	652607	1
Phönix	Lavender oil	652607	1
Phönix	Lavender oil		1
Anzag 17.08.2012	Lavender oil	680588	1
Caelo	Lavender oil	9229520	1
Caelo	Lavender oil	L12334511	1
Caelo	Lavender oil	13252224	1
Euro OTC	Lavender oil	1601053-01	1
Caelo	Lavender oil	15363002	1
Bombastus	Lavender oil	290711	1
Caelo	Lavender oil		1
Caelo	Lavender oil	15363305	1
Gehe	Lavender oil	11221301	1
Fiebig	Lavender oil	266070	1
Bombastus	Lavender oil	274960	1
Euro OTC	Lavender oil	1210031-01	1
Bombastus	Lavender oil	276644	1

- 57 897 spectra from 332 *Apo-Ident* customers from a total of 19 892 batches from a further 328 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 *Lavender oil* / *Clary 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 *Lavender oil* / *Clary 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	500	0	33 844
Type B	0	300	0	63 294
Type C	0	516	28	57 897

The substance/substance group *Lavender oil* / *Clary 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 % (> 99.9689 %)	100.0000 % (> 98.8000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.5963 %)	94.8529 % (> 94.3015 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30861	32710	16.52	59.72
31223	31223	0.00	59.20
31237	32710	16.54	66.90
31238	31721	2.42	56.78
31413	31413	0.00	62.81
31416	32710	17.25	61.27
31422	31223	2.01	59.08
31528	31528	0.00	63.09
31668	31413	6.49	66.15
31721	31721	0.00	59.76
31800	31800	0.00	58.08
32710	32710	0.00	61.55
32996	31721	3.77	51.56

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Liniment ointments
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30982-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Liniment ointments; Hydrated liniment SR/DAC (NRF p.40); Liniment, non-ionic hydrated DAC (NRF p.39.); Linimentum aquosum N (NRF S. 39); Linimentum aquosum SR/DAC (NRF S.40); Linimentum nonionicum aquosum DAC

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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
Leyh Pharma	Hydrated linimen...	124611	30982	80	20121123
Bombastus	Liniment, non-io...	282335	31169	40	1405256
apomix	Hydrated linimen...	73A041113	31170	40	1405106
Caelo	Hydrated linimen...	14063201	31438	40	20140513

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Liniment, non-io. . .	14134601	31476	40	20140516
Caelo	Liniment, non-io. . .	15420901	31827	40	20151221
Bombastus	Liniment, non-io. . .	297176	31830	40	20150909
Caelo	Hydrated linimen. . .	160217	31938	40	20160127*
Caelo	Hydrated linimen. . .	153244	31939	40	20150922*
Caelo	Liniment, non-io. . .	153267	31943	40	20150922*
Caelo	Liniment, non-io. . .	153342	31945	40	20151008*
Caelo	Liniment, non-io. . .	160216	31947	40	20160127*
Caelo	Liniment, non-io. . .	161138	32090	40	20160415*
apomix	Hydrated linimen. . .	08B010216	32305	40	20160203
apomix	Hydrated linimen. . .	32B090516	32727	40	20160509

Validation samples

A total of 156379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 640 spectra of 15 reference samples from the substance/substance group *Liniment ointments*. These samples are listed above in the [calibration samples](#) section.
- 33704 spectra from a total of 783 batches from further 223 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 1760 spectra of 46 reference samples from the substance/substance group *Liniment ointments*.

Supplier	Substance	Batch	Sample ID	Spectra
apomix	Hydrated liniment SR/DAC (NR. . .	105A291210	30240	80
Bombastus	Liniment, non-ionic hydrated. . .	253524	30282	40
Leyh Pharma	Hydrated liniment SR/DAC (NR. . .	111441	30283	40
Bombastus	Liniment, non-ionic hydrated. . .	262833	30332	40
Bombastus	Liniment, non-ionic hydrated. . .	262832	30338	40
apomix	Hydrated liniment SR/DAC (NR. . .	62B010811	30351	30
apomix	Liniment, non-ionic hydrated. . .	18A011111	30354	30
Caelo	Liniment, non-ionic hydrated. . .	15420901	31827 [†]	20
Bombastus	Liniment, non-ionic hydrated. . .	297176	31830 [†]	20

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

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrated liniment SR/DAC (NR...	160217	31938 [†]	20
Caelo	Hydrated liniment SR/DAC (NR...	153244	31939 [†]	20
Caelo	Liniment, non-ionic hydrated...	153267	31943 [†]	20
Caelo	Liniment, non-ionic hydrated...	153341	31944	60
Caelo	Liniment, non-ionic hydrated...	153342	31945 [†]	20
Caelo	Liniment, non-ionic hydrated...	153342	31946	60
Caelo	Liniment, non-ionic hydrated...	160216	31947 [†]	20
Caelo	Hydrated liniment SR/DAC (NR...	160217	32089	40
Caelo	Liniment, non-ionic hydrated...	161139	32091	40
Caelo	Liniment, non-ionic hydrated...	161140	32092	40
Caelo	Hydrated liniment SR/DAC (NR...	161824	32395	40
Caelo	Hydrated liniment SR/DAC (NR...	161824	32396	40
Caelo	Hydrated liniment SR/DAC (NR...	161824	32397	40
Caelo	Liniment, non-ionic hydrated...	161767	32398	40
Caelo	Liniment, non-ionic hydrated...	161767	32399	40
Caelo	Liniment, non-ionic hydrated...	161767	32400	40
Caelo	Liniment, non-ionic hydrated...	161768	32401	40
Caelo	Liniment, non-ionic hydrated...	161768	32402	40
Caelo	Liniment, non-ionic hydrated...	161768	32403	40
Caelo	Liniment, non-ionic hydrated...	162035	32404	40
Caelo	Liniment, non-ionic hydrated...	162035	32405	40
Caelo	Liniment, non-ionic hydrated...	161139	32604	40
Caelo	Liniment, non-ionic hydrated...	162181	32605	40
Caelo	Liniment, non-ionic hydrated...	162181	32606	40
Caelo	Liniment, non-ionic hydrated...	162181	32607	40
Caelo	Liniment, non-ionic hydrated...	162181	32608	40
Caelo	Liniment, non-ionic hydrated...	162182	32609	40
Caelo	Liniment, non-ionic hydrated...	162182	32610	40
Caelo	Liniment, non-ionic hydrated...	162183	32611	40
Caelo	Liniment, non-ionic hydrated...	162183	32612	40
Caelo	Liniment, non-ionic hydrated...	162183	32613	40
Caelo	Liniment, non-ionic hydrated...	162183	32614	40
Caelo	Liniment, non-ionic hydrated...	162584	32615	40
Caelo	Liniment, non-ionic hydrated...	162585	32616	40
Caelo	Liniment, non-ionic hydrated...	162585	32617	40
Caelo	Liniment, non-ionic hydrated...	162585	32618	40
Caelo	Liniment, non-ionic hydrated...	163188	32874	40

- 61 834 spectra from a total of 1450 batches from further 438 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.

- 1077 spectra from 161 *Apo-Ident* customers from 519 batches from the substance/substance group *Liniment ointments*.

[†]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*.

Supplier	Substance	Batch	Spectra
Apomix	Liniment, non-ionic hydrated...	23A111213	2
apomix	Hydrated liniment SR/DAC (NR...		1
Apomix	Hydrated liniment SR/DAC (NR...	5A210113	1
Apomix PKH GmbH	Liniment, non-ionic hydrated...	4A010316	1
PKH Halle / Phoenix	Hydrated liniment SR/DAC (NR...	2A120115	1
PKH Halle / Phoenix	Hydrated liniment SR/DAC (NR...	5A190115	1
Apomix	Hydrated liniment SR/DAC (NR...	3A070114	1
Gehe	Hydrated liniment SR/DAC (NR...	6B260115	1
Apomix	Hydrated liniment SR/DAC (NR...	3B130115	1
Apomix	Liniment, non-ionic hydrated...	10A310516	1
apomix/Holdermann	Hydrated liniment SR/DAC (NR...	9A020215	1
Apomix	Hydrated liniment SR/DAC (NR...	12B110214	1
Apomix	Hydrated liniment SR/DAC (NR...	13A110214	1
Leyh-Pharma GmbH	Hydrated liniment SR/DAC (NR...	133721	1
AHD/Leyh Pharma/25.10.14	Hydrated liniment SR/DAC (NR...	144031	1
Caelo	Liniment, non-ionic hydrated...	15192401	11
Leyh-Pharma GmbH	Hydrated liniment SR/DAC (NR...	142231	1
AHD/23.07.14/Leyh Pharma	Hydrated liniment SR/DAC (NR...	142231	1
Leyh Pharma / Alliance ...	Hydrated liniment SR/DAC (NR...	153511	1
PKH Halle	Liniment, non-ionic hydrated...	13A200616	1
Caelo	Liniment, non-ionic hydrated...	15326703	4
Caelo	Hydrated liniment SR/DAC (NR...	15324403	1
Leyh Phama	Hydrated liniment SR/DAC (NR...	154111	1
Caelo	Hydrated liniment SR/DAC (NR...	14350002	1
Pharmachem/Phönix	Hydrated liniment SR/DAC (NR...	160115	1
Leyhs Pharma GmbH	Hydrated liniment SR/DAC (NR...	161121	1
Caelo	Liniment, non-ionic hydrated...	16218201	5
Pharmachem/Phönix	Hydrated liniment SR/DAC (NR...	190416	1
Caelo	Liniment, non-ionic hydrated...	16114002	5
apomix	Hydrated liniment SR/DAC (NR...	17A290216	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	17A030314	1
Euro OTC	Liniment, non-ionic hydrated...	16C190716	1
Pharmachem GmbH Pößneck	Hydrated liniment SR/DAC (NR...	190416	1
Bombastus	Liniment, non-ionic hydrated...	192621	1
PKH Halle / Phoenix	Hydrated liniment SR/DAC (NR...	22A250314	1
Apomix	Hydrated liniment SR/DAC (NR...	22A250314	1
Apomix PKH GmbH	Liniment, non-ionic hydrated...	20A280915	1
apomix/Phönix	Hydrated liniment SR/DAC (NR...	22A250314	1
GEHE/Apomix/29.04.14	Hydrated liniment SR/DAC (NR...	24A310314	1
Apomix/ Phoenix	Liniment, non-ionic hydrated...	25A081215	1
Bombastus	Hydrated liniment SR/DAC (NR...	281644	1
Raben-Apotheke Mildenau	Hydrated liniment SR/DAC (NR...	25A310314	2
Bombastus	Hydrated liniment SR/DAC (NR...	284234	1
Bombastus	Hydrated liniment SR/DAC (NR...	285737	3
Bombastus	Liniment, non-ionic hydrated...	282947	4
Bombastus	Hydrated liniment SR/DAC (NR...	282885	2
Bombastus	Liniment, non-ionic hydrated...	282945	2
Bombastus	Hydrated liniment SR/DAC (NR...	284339	2
Bombastus	Hydrated liniment SR/DAC (NR...	285792	1
Bombastus	Hydrated liniment SR/DAC (NR...	285739	1
Bombastus	Hydrated liniment SR/DAC (NR...	285738	3
Bombastus	Liniment, non-ionic hydrated...	285793	5
Bombastus	Hydrated liniment SR/DAC (NR...	285838	1
Bombastus	Liniment, non-ionic hydrated...	286419	2
Bombastus	Liniment, non-ionic hydrated...	286418	8
Bombastus	Liniment, non-ionic hydrated...	286421	1
Phönix Gotha	Liniment, non-ionic hydrated...	287316	1
Bombastus	Liniment, non-ionic hydrated...	287318	6
Bombastus	Hydrated liniment SR/DAC (NR...	286935	3
Bombastus	Hydrated liniment SR/DAC (NR...	286936	2

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Supplier	Substance	Batch	Spectra
Bombastus	Liniment, non-ionic hydrated...	286417	5
Bombastus	Liniment, non-ionic hydrated...	287321	4
Bombastus	Hydrated liniment SR/DAC (NR...	287409	1
Bombastus	Liniment, non-ionic hydrated...	287323	3
Bombastus	Hydrated liniment SR/DAC (NR...	287410	3
Fagron	Liniment, non-ionic hydrated...	288452	1
Bombastus	Liniment, non-ionic hydrated...	288453	6
Bombastus	Liniment, non-ionic hydrated...	288391	1
Caelo	Liniment, non-ionic hydrated...	288454	1
Bombastus	Hydrated liniment SR/DAC (NR...	288535	6
Bombastus	Hydrated liniment SR/DAC (NR...	288533	1
Bombastus	Liniment, non-ionic hydrated...	289209	2
Gehe	Liniment, non-ionic hydrated...	289208	1
Bombastus	Liniment, non-ionic hydrated...	290121	2
Bombastus	Liniment, non-ionic hydrated...	291222	6
Phönix Gotha	Liniment, non-ionic hydrated...	290610	1
Bombastus	Liniment, non-ionic hydrated...	290613	5
Bombastus	Liniment, non-ionic hydrated...	291859	3
Bombastus	Liniment, non-ionic hydrated...	291860	3
Bombastus	Hydrated liniment SR/DAC (NR...	291866	1
Phönix Gotha	Liniment, non-ionic hydrated...	292617	1
Bombastus	Liniment, non-ionic hydrated...	292618	2
Bombastus	Hydrated liniment SR/DAC (NR...	294433	2
Bombastus	Hydrated liniment SR/DAC (NR...	292621	2
Bombastus	Liniment, non-ionic hydrated...	292742	1
Bombastus	Hydrated liniment SR/DAC (NR...	293590	4
Bombastus	Hydrated liniment SR/DAC (NR...	294434	2
Bombastus	Hydrated liniment SR/DAC (NR...	295854	2
Phönix Gotha	Liniment, non-ionic hydrated...	295072	1
Bombastus	Hydrated liniment SR/DAC (NR...	299988	1
Bombastus	Liniment, non-ionic hydrated...	296106	3
Bombastus	Hydrated liniment SR/DAC (NR...	296504	3
Bombastus	Hydrated liniment SR/DAC (NR...	295857	3
Phönix Gotha	Liniment, non-ionic hydrated...	296108	1
Bombastus	Hydrated liniment SR/DAC (NR...	299987	3
Bombastus	Liniment, non-ionic hydrated...	300195	4
PKH Halle / Noweda	Hydrated liniment SR/DAC (NR...	29A270415	1
Caelo	Liniment, non-ionic hydrated...	297171	1
Bombastus	Liniment, non-ionic hydrated...	300197	1
Bombastus	Liniment, non-ionic hydrated...	300864	4
Phoenix	Liniment, non-ionic hydrated...	300860	1
Bombastus	Liniment, non-ionic hydrated...	300863	2
Bombastus	Hydrated liniment SR/DAC (NR...	300967	1
Bombastus	Liniment, non-ionic hydrated...	301558	3
Bombastus	Hydrated liniment SR/DAC (NR...	300965	3
Ebert u. Jacobi 16.0...	Liniment, non-ionic hydrated...	300864	1
Bombastus	Hydrated liniment SR/DAC (NR...	302930	1
Bombastus	Hydrated liniment SR/DAC (NR...	302931	1
Bombastus	Hydrated liniment SR/DAC (NR...	302933	2
Bombastus	Hydrated liniment SR/DAC (NR...	300966	1
Bombastus	Hydrated liniment SR/DAC (NR...	300968	4
Bombastus	Hydrated liniment SR/DAC (NR...	301562	1
Bombastus	Liniment, non-ionic hydrated...	302287	1
Bombastus	Liniment, non-ionic hydrated...	302851	2
Bombastus	Hydrated liniment SR/DAC (NR...	3048843	1
Bombastus	Liniment, non-ionic hydrated...	305596	1
Bombastus	Liniment, non-ionic hydrated...	304933	1
apomix/Holdermann	Hydrated liniment SR/DAC (NR...	35A170516	1
apomix GmbH/Phönix	Hydrated liniment SR/DAC (NR...	36A120514	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	41A260514	1

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Supplier	Substance	Batch	Spectra
apomix PKH GmbH Halle	Hydrated liniment SR/DAC (NR...	41A080615	1
apomix	Hydrated liniment SR/DAC (NR...	36A120514	1
Gehe/18.08.14	Hydrated liniment SR/DAC (NR...	42A020614	3
PKH Halle	Hydrated liniment SR/DAC (NR...	42A020614	1
PKH Halle / Phoenix	Hydrated liniment SR/DAC (NR...	45A170614	1
Apomix	Hydrated liniment SR/DAC (NR...	45A170614	1
apomix	Hydrated liniment SR/DAC (NR...	46A290615	1
Gehe	Hydrated liniment SR/DAC (NR...	46B260514	2
Apomix/Phönix	Hydrated liniment SR/DAC (NR...	47B170614	1
AMH Niemann/Sanacorp	Hydrated liniment SR/DAC (NR...	46B260514	1
Bombastus	Liniment, non-ionic hydrated...	488451	1
Apomix/Sanacorp	Hydrated liniment SR/DAC (NR...	55A040815	1
Gehe	Hydrated liniment SR/DAC (NR...	50B300614	1
Apomix/Phönix	Hydrated liniment SR/DAC (NR...	59A050814	1
apomix	Hydrated liniment SR/DAC (NR...	63A120814	1
Apomix/NOWEDA	Hydrated liniment SR/DAC (NR...	54A030815	1
Apomix	Hydrated liniment SR/DAC (NR...	64A140915	1
apomix	Hydrated liniment SR/DAC (NR...	55A250716	1
PKH Halle / Phoenix	Hydrated liniment SR/DAC (NR...	59A050814	1
apomix/Gehe	Hydrated liniment SR/DAC (NR...	68A080914	1
Gehe 09.01.15 Apomix	Hydrated liniment SR/DAC (NR...	67A010914	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	67A010914	1
PKH Halle	Hydrated liniment SR/DAC (NR...	69A080914	1
Apomix / Phönix	Hydrated liniment SR/DAC (NR...	69B071013	2
Apomix	Hydrated liniment SR/DAC (NR...	72B041113	1
Gehe 09.01.15/apomix	Hydrated liniment SR/DAC (NR...	74A131014	1
Gehe/apomix/12.03.14	Hydrated liniment SR/DAC (NR...	79A091213	1
Rabenapotheke	Hydrated liniment SR/DAC (NR...	76A271014	1
Apomix	Hydrated liniment SR/DAC (NR...	80A241114	1
Phönix	Hydrated liniment SR/DAC (NR...		1
Apomix/Gehe/12.05.14	Hydrated liniment SR/DAC (NR...	81A161213	1
Phönix Gotha	Liniment, non-ionic hydrated...	264180	1
apomix	Hydrated liniment SR/DAC (NR...	88A161214	1
ANZAG am 23.04.2012	Liniment, non-ionic hydrated...	269132	1
Bombastus	Liniment, non-ionic hydrated...	264181	1
Bombastus	Liniment, non-ionic hydrated...	269133	1
Bombastus	Liniment, non-ionic hydrated...	268125	1
Bombastus	Liniment, non-ionic hydrated...	269843	1
Caelo	Liniment, non-ionic hydrated...	269134	1
Gehe	Liniment, non-ionic hydrated...	269845	1
Noweda	Liniment, non-ionic hydrated...	269847	1
Noweda	Liniment, non-ionic hydrated...	269848	1
Noweda	Liniment, non-ionic hydrated...	271243	1
Phönix Gotha	Liniment, non-ionic hydrated...	270007	2
Bombastus	Liniment, non-ionic hydrated...	269847	1
Bombastus	Liniment, non-ionic hydrated...	271245	2
Bombastus	Liniment, non-ionic hydrated...	271249	1
Gehe	Liniment, non-ionic hydrated...	271305	1
Gehe	Liniment, non-ionic hydrated...	272611	2
Phönix Gotha	Liniment, non-ionic hydrated...	273375	2
Phoenix, 12.09.2012	Liniment, non-ionic hydrated...	271302	1
Bombastus	Liniment, non-ionic hydrated...	272614	1
Apomix/ Phönix	Liniment, non-ionic hydrated...	11A010713	1
Gehe	Liniment, non-ionic hydrated...	274014	1
apomix/Phönix	Liniment, non-ionic hydrated...	17A030912	2
Bombastus	Liniment, non-ionic hydrated...	274016	2
Apomix/Phönix	Liniment, non-ionic hydrated...	9A290513	1
Pharmachem / Anzag	Liniment, non-ionic hydrated...	250512	1
Apomix	Liniment, non-ionic hydrated...	24A101212	1
Caelo	Liniment, non-ionic hydrated...	16113901	3

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Supplier	Substance	Batch	Spectra
Apomix / Phönix	Liniment, non-ionic hydrated...	20A051113	1
PKH Halle / Phoenix	Liniment, non-ionic hydrated...	17A230913	1
Bombastus	Liniment, non-ionic hydrated...	270673	2
Sanacorp	Liniment, non-ionic hydrated...	274820	1
Bombastus	Liniment, non-ionic hydrated...	275626	1
Bombastus	Liniment, non-ionic hydrated...	275788	5
Bombastus	Liniment, non-ionic hydrated...	278256	1
Phönix 05.04.2013	Liniment, non-ionic hydrated...	275787	1
Bombastus	Liniment, non-ionic hydrated...	280876	2
Bombastus	Liniment, non-ionic hydrated...	275785	2
Caelo	Liniment, non-ionic hydrated...	281564	2
Bombastus	Liniment, non-ionic hydrated...	282332	3
Bom/Kehr	Liniment, non-ionic hydrated...	282332	1
Bombastus	Liniment, non-ionic hydrated...	276525	3
Phönix Gotha	Liniment, non-ionic hydrated...	281559	2
Bombastus	Liniment, non-ionic hydrated...	279502	4
Bombastus	Hydrated liniment SR/DAC (NR...	268572	1
Bombastus	Hydrated liniment SR/DAC (NR...	266553	1
Bombastus	Hydrated liniment SR/DAC (NR...	268577	2
Bombastus	Hydrated liniment SR/DAC (NR...	269848	1
Gehe	Hydrated liniment SR/DAC (NR...	269845	1
Bombastus	Hydrated liniment SR/DAC (NR...	273772	2
Bombastus	Hydrated liniment SR/DAC (NR...	270480	1
Bombastus	Hydrated liniment SR/DAC (NR...	270479	1
Bombastus	Hydrated liniment SR/DAC (NR...	272646	1
Bombastus	Liniment, non-ionic hydrated...	272615	4
Bombastus	Hydrated liniment SR/DAC (NR...	273774	3
Phönix Gotha	Hydrated liniment SR/DAC (NR...	274014	1
Bombastus	Liniment, non-ionic hydrated...	274014	2
Bombastus	Liniment, non-ionic hydrated...	274015	1
Noweda	Liniment, non-ionic hydrated...	274016	1
Pharmachem/Phönix	Hydrated liniment SR/DAC (NR...	21013	1
Sanacorp/ Leyh Pharma	Hydrated liniment SR/DAC (NR...	115051	1
PKH Halle	Liniment, non-ionic hydrated...	6A120312	1
Angag Leyh	Hydrated liniment SR/DAC (NR...	4580715	1
apomix/Phönix	Hydrated liniment SR/DAC (NR...	5A210113	1
Anzag	Liniment, non-ionic hydrated...	91012	1
Apomix	Hydrated liniment SR/DAC (NR...	10A260213	1
Apomix	Hydrated liniment SR/DAC (NR...	6A2000114	1
Leyh Pharma	Hydrated liniment SR/DAC (NR...	122141	1
Sanacorp/ Leyh Pharma	Hydrated liniment SR/DAC (NR...	122141	1
Leyh Pharma	Hydrated liniment SR/DAC (NR...	122531	4
Sanacorp/ Leyh Pharma	Hydrated liniment SR/DAC (NR...	123011	1
Leyh Pharma	Hydrated liniment SR/DAC (NR...	123621	1
Leyh Pharma	Hydrated liniment SR/DAC (NR...	124941	1
leyh Pharma/ Sanacorp	Hydrated liniment SR/DAC (NR...	124941	1
Leyh/Gehe	Hydrated liniment SR/DAC (NR...	131121	1
Apomix/Phönix	Hydrated liniment SR/DAC (NR...	15A260813	2
PKH Halle / Phoenix	Hydrated liniment SR/DAC (NR...	15A050313	1
pkh, Phönix	Hydrated liniment SR/DAC (NR...	14B170214	1
Leyh	Hydrated liniment SR/DAC (NR...	124941	1
Apomix	Hydrated liniment SR/DAC (NR...	20B180313	1
Apomix	Hydrated liniment SR/DAC (NR...	16A070312	2
Apomix	Liniment, non-ionic hydrated...	17A030912	1
Pharmachem/ANZAG/27.03...	Hydrated liniment SR/DAC (NR...	210113	1
Bombastus	Liniment, non-ionic hydrated...	274869	1
apomix	Hydrated liniment SR/DAC (NR...	23A020413	1
Noweda	Liniment, non-ionic hydrated...	275786	1
Bombastus	Hydrated liniment SR/DAC (NR...	275792	1
Bombastus	Hydrated liniment SR/DAC (NR...	274772	2

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Supplier	Substance	Batch	Spectra
Bombastus	Liniment, non-ionic hydrated...	275787	2
Phönix Gotha	Hydrated liniment SR/DAC (NR...	275789	1
PKH GmbH/ Phönix	Hydrated liniment SR/DAC (NR...	23A020413	1
Phönix Gotha	Liniment, non-ionic hydrated...	275792	1
Bombastus	Hydrated liniment SR/DAC (NR...	277781	2
Bombastus	Hydrated liniment SR/DAC (NR...	279398	2
Bombastus	Hydrated liniment SR/DAC (NR...	275864	1
Bombastus	Hydrated liniment SR/DAC (NR...	275869	1
Phönix Gotha	Hydrated liniment SR/DAC (NR...	279496	1
Bombastus	Hydrated liniment SR/DAC (NR...	279400	2
Apomix	Hydrated liniment SR/DAC (NR...	27A230413	1
Bombastus	Hydrated liniment SR/DAC (NR...	280805	2
Bombstus/ Sanacorp	Hydrated liniment SR/DAC (NR...	281643	2
Bombastus	Hydrated liniment SR/DAC (NR...	281562	1
Bombastus	Hydrated liniment SR/DAC (NR...	281642	3
Bombastus	Hydrated liniment SR/DAC (NR...	281645	2
Apomix/Kehr	Hydrated liniment SR/DAC (NR...	29A060513	1
Anzag	Hydrated liniment SR/DAC (NR...	30B130513	1
Euro OTC	Hydrated liniment SR/DAC (NR...	33A210513	1
pkh, Phönix	Hydrated liniment SR/DAC (NR...	32A120515	1
apomix	Hydrated liniment SR/DAC (NR...	33A210513	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	40A170613	1
Apomix / Phönix	Hydrated liniment SR/DAC (NR...	38A040613	1
Apomix	Hydrated liniment SR/DAC (NR...	42B240613	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	43A010713	1
Apomix/Phoenix	Hydrated liniment SR/DAC (NR...	51A230713	1
Caelo	Hydrated liniment SR/DAC (NR...	47B020712	1
PKH Halle	Hydrated liniment SR/DAC (NR...	56A120813	4
PHK GmbH	Hydrated liniment SR/DAC (NR...	66A160913	1
apomix/Phönix	Hydrated liniment SR/DAC (NR...	68A300913	1
Apomix	Hydrated liniment SR/DAC (NR...	62B050913	1
Apomix	Hydrated liniment SR/DAC (NR...	70A071013	2
PKH Halle / Phoenix	Hydrated liniment SR/DAC (NR...	71A291013	2
PHK GmbH	Hydrated liniment SR/DAC (NR...	71A291013	2
Phoenix/Apomix	Hydrated liniment SR/DAC (NR...	71A291013	1
Caelo	Hydrated liniment SR/DAC (NR...	74B081012	2
Gehe/Apomix	Hydrated liniment SR/DAC (NR...	77A251113	1
Apomix	Hydrated liniment SR/DAC (NR...	79A091213	2
Apomix/Gehe	Hydrated liniment SR/DAC (NR...	85A281112	1
Apomix	Hydrated liniment SR/DAC (NR...	83A071112	1
PKH GmbH / Phönix	Liniment, non-ionic hydrated...	11B270515	1
Caelo	Liniment, non-ionic hydrated...	15014601	6
Caelo	Liniment, non-ionic hydrated...	15096101	7
Caelo	Liniment, non-ionic hydrated...	15192502	7
Caelo	Liniment, non-ionic hydrated...	15096002	2
Caelo	Liniment, non-ionic hydrated...	15192301	6
Caelo	Liniment, non-ionic hydrated...	16021601	7
Caelo	Liniment, non-ionic hydrated...	16176802	1
Caelo	Liniment, non-ionic hydrated...	16218301	1
Bombastus	Liniment, non-ionic hydrated...	285025	2
Bombastus	Hydrated liniment SR/DAC (NR...	285740	1
Bombastus	Liniment, non-ionic hydrated...	288451	5
Bombastus	Hydrated liniment SR/DAC (NR...	288536	1
Bombastus	Hydrated liniment SR/DAC (NR...	288538	1
Bombastus	Liniment, non-ionic hydrated...	290612	2
Bombastus	Hydrated liniment SR/DAC (NR...	289863	2
Bombastus	Liniment, non-ionic hydrated...	291223	2
Bombastus	Liniment, non-ionic hydrated...	291286	2
Bombastus	Hydrated liniment SR/DAC (NR...	292493	3
Bombastus	Liniment, non-ionic hydrated...	295069	1

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Supplier	Substance	Batch	Spectra
Bombastus	Hydrated liniment SR/DAC (NR...	294435	1
Bombastus	Liniment, non-ionic hydrated...	295073	1
Bombastus	Liniment, non-ionic hydrated...	267329	1
Bombastus	Liniment, non-ionic hydrated...	269131	1
Anzag	Liniment, non-ionic hydrated...	274016	1
Bombastus	Liniment, non-ionic hydrated...	271236	1
Bombastus	Liniment, non-ionic hydrated...	273371	1
Bombastus	Liniment, non-ionic hydrated...	274819	2
Bombastus	Liniment, non-ionic hydrated...	274813	1
Gehe	Liniment, non-ionic hydrated...	275792	1
Gehe	Liniment, non-ionic hydrated...	279498	2
Gehe	Liniment, non-ionic hydrated...	289205	1
Bombastus	Liniment, non-ionic hydrated...	287320	1
	Liniment, non-ionic hydrated...	288452	1
Bombastus	Hydrated liniment SR/DAC (NR...	265946	1
Bombastus	Hydrated liniment SR/DAC (NR...	273773	1
Bombastus	Hydrated liniment SR/DAC (NR...	270673	1
Sanacorp	Hydrated liniment SR/DAC (NR...	275869	1
Bombastus	Hydrated liniment SR/DAC (NR...	279399	1
PKH GmbH/ Sanacorp	Hydrated liniment SR/DAC (NR...	78B031213	1
Bombastus	Liniment, non-ionic hydrated...	276523	1
Sanacorp	Liniment, non-ionic hydrated...	279500	1
Bombastus	Liniment, non-ionic hydrated...	281563	2
Bombastus	Liniment, non-ionic hydrated...	279501	4
Bombastus	Liniment, non-ionic hydrated...	282334	4
Anzag	Liniment, non-ionic hydrated...	275786	1
Gehe Kassel	Liniment, non-ionic hydrated...	15014601	2
Apomix	Liniment, non-ionic hydrated...	2A020216	2
apomix	Liniment, non-ionic hydrated...	3A100215	1
Apomix/Noweda	Liniment, non-ionic hydrated...	3B180214	1
PKH Halle / Phoenix	Liniment, non-ionic hydrated...	4A250214	1
Apomix	Liniment, non-ionic hydrated...	4A250214	1
Apomix	Liniment, non-ionic hydrated...	5A110315	1
apomix/Phönix	Liniment, non-ionic hydrated...	5B170414	2
Apomix	Liniment, non-ionic hydrated...	6A310316	1
Apomix/Noweda	Liniment, non-ionic hydrated...	6B180315	1
Apomix	Liniment, non-ionic hydrated...	7A170414	1
apomix/Phönix	Liniment, non-ionic hydrated...	8A080415	1
Apomix	Liniment, non-ionic hydrated...	9A190516	1
Caelo	Liniment, non-ionic hydrated...	102600630	1
apomix PKH GmbH Halle	Liniment, non-ionic hydrated...	9A190516	1
AHD 09.01.15/apomix	Liniment, non-ionic hydrated...	A150914	1
Caelo	Liniment, non-ionic hydrated...	10A310516	1
PKH Halle / Phoenix	Liniment, non-ionic hydrated...	10A150514	1
Caelo	Liniment, non-ionic hydrated...	10A110515	1
Noweda/apomix	Liniment, non-ionic hydrated...	12A100615	1
apomix	Liniment, non-ionic hydrated...	12A100615	1
Apomix	Liniment, non-ionic hydrated...	12A270514	1
apomix	Liniment, non-ionic hydrated...	13A040614	1
Apomix/Noweda	Liniment, non-ionic hydrated...	13A040614	1
Caelo	Liniment, non-ionic hydrated...	14092015A	1
Caelo	Liniment, non-ionic hydrated...	14134601	5
Alliance Health 09.05.2...	Liniment, non-ionic hydrated...	14134601	2
Caelo	Liniment, non-ionic hydrated...	14173601	1
Caelo	Liniment, non-ionic hydrated...	14209501	7
Caelo	Liniment, non-ionic hydrated...	14276002	5
Caelo	Liniment, non-ionic hydrated...	14328402	1
Caelo	Liniment, non-ionic hydrated...	14350703	1
Alliance health	Liniment, non-ionic hydrated...	14350703	2
Fagron	Liniment, non-ionic hydrated...	14350703	1

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Supplier	Substance	Batch	Spectra
Caelo	Liniment, non-ionic hydrated...	15002302	1
Sanacorp	Liniment, non-ionic hydrated...	15002302	1
Noweda	Liniment, non-ionic hydrated...	15096002	3
Cealo/Noweda	Liniment, non-ionic hydrated...	15096101	1
Noweda 27.08.15	Liniment, non-ionic hydrated...	15192301	1
Caelo	Liniment, non-ionic hydrated...	15326702	6
PKH Halle / Phoenix	Liniment, non-ionic hydrated...	15A140714	1
Noweda	Liniment, non-ionic hydrated...	15421002	1
Caelo	Liniment, non-ionic hydrated...	15420901	2
apomix	Liniment, non-ionic hydrated...	15A150715	2
PKH Halle / Phoenix	Liniment, non-ionic hydrated...	15A150715	1
Noweda	Liniment, non-ionic hydrated...	15420902	1
Caelo	Liniment, non-ionic hydrated...	16113801	4
Caelo	Liniment, non-ionic hydrated...	16113902	1
Caelo	Liniment, non-ionic hydrated...	16176701	7
Apomix	Liniment, non-ionic hydrated...	16A040814	1
Apomix	Liniment, non-ionic hydrated...	16A050815	2
Apomix	Liniment, non-ionic hydrated...	18A200814	1
Apomix	Liniment, non-ionic hydrated...	19A010916	1
AHD 09.01.15/apomix	Liniment, non-ionic hydrated...	20A150914	1
apomix	Liniment, non-ionic hydrated...	20A280915	1
PKH GmbH	Liniment, non-ionic hydrated...	21A241016	1
Apomix	Liniment, non-ionic hydrated...	22A101114	2
apomix/Phönix	Liniment, non-ionic hydrated...	22A101114	1
PKH GmbH	Liniment, non-ionic hydrated...	22A251016	1
AHD 09.01.15/apomix	Liniment, non-ionic hydrated...	22A101114	1
Apomix	Liniment, non-ionic hydrated...	25A021214	2
PKH Halle / Phoenix	Liniment, non-ionic hydrated...	25A021214	1
Apomix	Liniment, non-ionic hydrated...	25A081215	1
Apomix / Phönix	Liniment, non-ionic hydrated...	25A191213	3
Apomix	Liniment, non-ionic hydrated...	27A221214	1
Apomix/Gehe	Liniment, non-ionic hydrated...	27A221214	1
Caelo	Liniment, non-ionic hydrated...	281562	1
Bombastus	Liniment, non-ionic hydrated...	282333	4
gehe	Liniment, non-ionic hydrated...	281560	2
Caelo	Liniment, non-ionic hydrated...	282946	1
Bombastus	Liniment, non-ionic hydrated...	285023	1
Caelo	Liniment, non-ionic hydrated...	285025	1
Bombastu-Werke AG/Gehe	Liniment, non-ionic hydrated...	285025	1
Bombastus	Liniment, non-ionic hydrated...	285024	1
Bombastus	Liniment, non-ionic hydrated...	285790	2
Bombastus	Liniment, non-ionic hydrated...	285792	2
Wolf-Apotheke	Liniment, non-ionic hydrated...	285793	1
gehe	Liniment, non-ionic hydrated...	285793	1
Bombastus	Liniment, non-ionic hydrated...	285795	3
Noweda	Liniment, non-ionic hydrated...	285795	1
Bombastus	Liniment, non-ionic hydrated...	285838	1
Gehe/Apomix	Liniment, non-ionic hydrated...	286417	1
Gehe	Liniment, non-ionic hydrated...	287316	1
Bombastus	Liniment, non-ionic hydrated...	287319	2
Gehe	Liniment, non-ionic hydrated...	286421	1
Caelo	Liniment, non-ionic hydrated...	287323	1
Noweda	Liniment, non-ionic hydrated...	287323	1
Bombastus	Liniment, non-ionic hydrated...	288387	1
Bombastus	Liniment, non-ionic hydrated...	288386	1
Gehe 18.08.14	Liniment, non-ionic hydrated...	288387	4
Bombastus	Liniment, non-ionic hydrated...	288389	1
Gehe	Liniment, non-ionic hydrated...	288387	1
Bombastus	Liniment, non-ionic hydrated...	288390	1
Bombastu-Werke AG/Gehe	Liniment, non-ionic hydrated...	288452	1

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Supplier	Substance	Batch	Spectra
Bombastus	Liniment, non-ionic hydrated...	288452	1
Bombastus	Liniment, non-ionic hydrated...	288454	3
Bombastus	Liniment, non-ionic hydrated...	289206	2
Bombastus	Liniment, non-ionic hydrated...	289205	1
Bombastus	Liniment, non-ionic hydrated...	289208	2
Bombastus	Liniment, non-ionic hydrated...	289207	1
Bomastus/Phönix	Liniment, non-ionic hydrated...	290610	1
Bombastus	Liniment, non-ionic hydrated...	291220	1
Bombastus	Liniment, non-ionic hydrated...	291221	2
Caelo	Liniment, non-ionic hydrated...	291222	1
Caelo	Liniment, non-ionic hydrated...	291286	1
Bombastus	Liniment, non-ionic hydrated...	291861	3
Bombastus	Liniment, non-ionic hydrated...	292617	1
Bombastus	Liniment, non-ionic hydrated...	292621	2
Caelo	Liniment, non-ionic hydrated...	292742	1
Bombastus	Liniment, non-ionic hydrated...	293578	2
Bombastus	Liniment, non-ionic hydrated...	293577	2
Bombastus	Liniment, non-ionic hydrated...	293579	5
Caelo	Liniment, non-ionic hydrated...	293579	1
Caelo	Liniment, non-ionic hydrated...	294211	2
Bombastus	Liniment, non-ionic hydrated...	294211	5
Bombastus	Liniment, non-ionic hydrated...	294212	1
Bombastus	Liniment, non-ionic hydrated...	294213	1
Bombastus	Liniment, non-ionic hydrated...	294277	1
Bombastus	Liniment, non-ionic hydrated...	295068	1
Bombastus	Liniment, non-ionic hydrated...	295070	6
Bombastus	Liniment, non-ionic hydrated...	295071	1
Bombastus	Liniment, non-ionic hydrated...	295072	1
Caelo	Liniment, non-ionic hydrated...	295072	1
Bombastus	Liniment, non-ionic hydrated...	295910	2
Caelo	Liniment, non-ionic hydrated...	295910	1
Bombastus	Liniment, non-ionic hydrated...		2
Bombastus	Liniment, non-ionic hydrated...	296109	1
Bombastus	Liniment, non-ionic hydrated...	296110	1
Bombastus	Liniment, non-ionic hydrated...	296107	2
Bombastus	Liniment, non-ionic hydrated...	296111	1
Caelo	Liniment, non-ionic hydrated...	296584	4
Bombastus	Liniment, non-ionic hydrated...	296584	1
Bombastus	Liniment, non-ionic hydrated...	296585	5
Bombastus	Liniment, non-ionic hydrated...	296589	3
Bombastus	Liniment, non-ionic hydrated...	297172	2
Bombastus	Liniment, non-ionic hydrated...	297173	2
Bombastus	Liniment, non-ionic hydrated...	297171	1
Bombastus	Liniment, non-ionic hydrated...	297174	2
Bombastus	Liniment, non-ionic hydrated...	297175	2
Rondell Apotheke	Liniment, non-ionic hydrated...	297175	1
Bombastus	Liniment, non-ionic hydrated...	297176	1
Bombastus	Liniment, non-ionic hydrated...	297177	3
Bombastus	Liniment, non-ionic hydrated...	297178	4
Caelo	Liniment, non-ionic hydrated...	297178	1
Bombastus	Liniment, non-ionic hydrated...	298465	2
Bombastus	Liniment, non-ionic hydrated...	298466	1
Caelo	Liniment, non-ionic hydrated...	298466	1
Bombastus	Liniment, non-ionic hydrated...	299133	1
Bombastus	Liniment, non-ionic hydrated...	300199	2
Caelo	Liniment, non-ionic hydrated...	300199	2
Bombastus	Liniment, non-ionic hydrated...	300200	3
Bombastus	Liniment, non-ionic hydrated...	300859	3
Bombastus	Liniment, non-ionic hydrated...	300860	2
Bombastus	Liniment, non-ionic hydrated...	300862	1

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Supplier	Substance	Batch	Spectra
Caelo	Liniment, non-ionic hydrated...	300864	2
Bombastus	Liniment, non-ionic hydrated...	301556	1
Bombastus	Liniment, non-ionic hydrated...	301557	2
Caelo	Liniment, non-ionic hydrated...	302283	1
Phoenix	Liniment, non-ionic hydrated...	302283	1
Bombastus	Liniment, non-ionic hydrated...	302284	1
Bombastus	Liniment, non-ionic hydrated...	302285	2
Bombastus	Liniment, non-ionic hydrated...	302286	1
Bombastus	Liniment, non-ionic hydrated...	302849	1
Bombastus	Liniment, non-ionic hydrated...	302852	2
Bombastus	Liniment, non-ionic hydrated...	303895	2
Phoenix	Liniment, non-ionic hydrated...	303895	1
Bombastus	Liniment, non-ionic hydrated...	304935	2
Bombastus	Liniment, non-ionic hydrated...	305595	1
Caelo	Liniment, non-ionic hydrated...	4063101	1
Bombastus	Liniment, non-ionic hydrated...	60091111	1
Bombastus	Liniment, non-ionic hydrated...	229263	1
Bombastus	Liniment, non-ionic hydrated...	267339	1
Bombastus	Liniment, non-ionic hydrated...	268124	1
Gehe	Liniment, non-ionic hydrated...	269846	1
Bombastus	Liniment, non-ionic hydrated...	269846	1
Gehe	Liniment, non-ionic hydrated...	271303	1
Bombastus	Liniment, non-ionic hydrated...	273373	1
Bombastus	Liniment, non-ionic hydrated...	273374	1
Fagron	Liniment, non-ionic hydrated...	27301	1
PKH Halle / Phoenix	Liniment, non-ionic hydrated...	4A110313	1
apomix	Liniment, non-ionic hydrated...	8A170412	1
Bombastus	Liniment, non-ionic hydrated...	7021402	1
apomix	Liniment, non-ionic hydrated...	10A1206013	1
Apomix	Liniment, non-ionic hydrated...	11A010713	1
apomix	Liniment, non-ionic hydrated...	11A010713	1
Fagron	Liniment, non-ionic hydrated...	122304	1
Caelo	Liniment, non-ionic hydrated...	123304	1
Fagron	Liniment, non-ionic hydrated...	123304	2
Apomix/Noweda	Liniment, non-ionic hydrated...	12A100713	1
Bombastus	Liniment, non-ionic hydrated...	131648	1
Caelo	Liniment, non-ionic hydrated...	14024104	1
Pharmachem / Anzag	Liniment, non-ionic hydrated...	150213	1
Phönix/Apomix	Liniment, non-ionic hydrated...	15A260813	1
Phönix (PKH Halle)	Liniment, non-ionic hydrated...	16A060812	1
Apomix	Liniment, non-ionic hydrated...	15A260813	1
PKH Halle,Phönix	Liniment, non-ionic hydrated...	17A030912	1
Apomix	Liniment, non-ionic hydrated...	15A300712	1
Apomix	Liniment, non-ionic hydrated...	17A230913	1
Apomix / Phönix	Liniment, non-ionic hydrated...	17A230913	1
Selbsthersteller	Liniment, non-ionic hydrated...	20140116	1
Caelo	Liniment, non-ionic hydrated...	2/AD1	1
PKH Halle,Anzag	Liniment, non-ionic hydrated...	20A221012	1
apomix	Liniment, non-ionic hydrated...	20A051113	1
Apomix / Phönix	Liniment, non-ionic hydrated...	23A111213	1
Caelo	Liniment, non-ionic hydrated...	21A201113	1
apomix	Liniment, non-ionic hydrated...	20A221012	1
apomix/Phönix	Liniment, non-ionic hydrated...	20A121211	1
apomix	Liniment, non-ionic hydrated...	24A101212	1
Fagron	Liniment, non-ionic hydrated...	258210	1
Fagron	Liniment, non-ionic hydrated...	257210	1
Bombastus	Liniment, non-ionic hydrated...	274815	1
Noweda	Liniment, non-ionic hydrated...	274820	2
Bombastus	Liniment, non-ionic hydrated...	274820	1
Phoenix am 07.03.2013	Liniment, non-ionic hydrated...	275785	2

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Supplier	Substance	Batch	Spectra
Bombastus	Liniment, non-ionic hydrated...	275786	4
Caelo	Liniment, non-ionic hydrated...	275787	1
Anzag	Liniment, non-ionic hydrated...	275788	1
Bombastus	Liniment, non-ionic hydrated...	275789	1
Gehe	Liniment, non-ionic hydrated...	275791	1
Bombastus	Liniment, non-ionic hydrated...	275792	1
Noweda	Liniment, non-ionic hydrated...	276525	2
Bombastus	Liniment, non-ionic hydrated...	276526	2
Gehe	Liniment, non-ionic hydrated...	276524	1
Gehe	Liniment, non-ionic hydrated...	278253	2
Phönix Gotha	Liniment, non-ionic hydrated...	278255	1
Bombastus	Liniment, non-ionic hydrated...	278258	4
Bombastus	Liniment, non-ionic hydrated...	278259	6
Bombastus	Liniment, non-ionic hydrated...	278260	3
Caesar & Loretz/ Noweda	Liniment, non-ionic hydrated...	278260	1
Caelo	Liniment, non-ionic hydrated...	278260	1
Bombastus	Liniment, non-ionic hydrated...	279496	1
Bombastus	Liniment, non-ionic hydrated...	279498	2
Bombastus	Liniment, non-ionic hydrated...	279497	1
Bombastus	Liniment, non-ionic hydrated...	279499	3
Sanacorp	Liniment, non-ionic hydrated...	279501	1
Bombastus	Liniment, non-ionic hydrated...	279500	2
post apotheke	Liniment, non-ionic hydrated...	279502	2
Gehe	Liniment, non-ionic hydrated...	280873	1
Bombastus	Liniment, non-ionic hydrated...	280877	6
Gehe	Liniment, non-ionic hydrated...	280877	1
Bombastus	Liniment, non-ionic hydrated...	281558	2
Bombastus	Liniment, non-ionic hydrated...	281561	2
Bombastus	Liniment, non-ionic hydrated...	281560	1
Bombastus	Liniment, non-ionic hydrated...	281562	2
Noweda	Liniment, non-ionic hydrated...	281562	1
/Noweda	Liniment, non-ionic hydrated...	281562	1
Gehe	Liniment, non-ionic hydrated...	281563	1
Bombastus	Liniment, non-ionic hydrated...	281564	4
Bombastu-Werke AG/Gehe	Liniment, non-ionic hydrated...	281564	1
Caelo	Liniment, non-ionic hydrated...	282333	1
Gehe	Liniment, non-ionic hydrated...	282335	1
Bombastus	Liniment, non-ionic hydrated...	282946	2
Phönix Gotha	Liniment, non-ionic hydrated...	282946	1
gehe	Liniment, non-ionic hydrated...	282947	1
Bombastu-Werke AG/Gehe	Liniment, non-ionic hydrated...	282947	1
Bombastus	Liniment, non-ionic hydrated...	284231	1
Bombastus	Liniment, non-ionic hydrated...	284234	1
Bombastus	Liniment, non-ionic hydrated...	284233	1
Bombastus	Liniment, non-ionic hydrated...	284237	1
Bombastus	Liniment, non-ionic hydrated...	284236	1
Bombastus	Liniment, non-ionic hydrated...	600991111	1
Pharmachem GmbH/Phönix	Hydrated liniment SR/DAC (NR...	30815	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	3A070114	1
apomix	Hydrated liniment SR/DAC (NR...	2A120115	1
Bombastus	Hydrated liniment SR/DAC (NR...	4A070114	1
Apomix	Hydrated liniment SR/DAC (NR...	6A200114	1
Apomix	Hydrated liniment SR/DAC (NR...	9A270114	1
apomix/Phönix	Hydrated liniment SR/DAC (NR...	10A080216	1
Euro Pharmachem/Phönix	Hydrated liniment SR/DAC (NR...	110315	1
Apomix / Phönix	Hydrated liniment SR/DAC (NR...	12B110214	1
apomix	Hydrated liniment SR/DAC (NR...	13A110214	2
GEHE/LEYH Parma/09.04.2...	Hydrated liniment SR/DAC (NR...	134211	2
PKH / Phoenix Leipzig	Hydrated liniment SR/DAC (NR...	14A040315	1
apomix	Hydrated liniment SR/DAC (NR...	19A070316	1

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Supplier	Substance	Batch	Spectra
apomix PKH GmbH Halle	Hydrated liniment SR/DAC (NR...	19B100314	1
Gehe/Apomix	Hydrated liniment SR/DAC (NR...	20A170315	1
PKH Halle	Hydrated liniment SR/DAC (NR...	24A310314	1
AMH Niemann/Noweda	Hydrated liniment SR/DAC (NR...	26A130415	1
Bombastus	Hydrated liniment SR/DAC (NR...	287323	1
Bombastus	Hydrated liniment SR/DAC (NR...	289862	1
Bombastus	Hydrated liniment SR/DAC (NR...	289864	1
apomix PKH GmbH Halle	Hydrated liniment SR/DAC (NR...	28A060416	1
Bombastus	Hydrated liniment SR/DAC (NR...	291867	1
Bombastus	Hydrated liniment SR/DAC (NR...	292491	3
Bombastus	Hydrated liniment SR/DAC (NR...	293591	1
Bombastus	Hydrated liniment SR/DAC (NR...	295852	1
Bombastus	Hydrated liniment SR/DAC (NR...	296506	1
Bombastus	Hydrated liniment SR/DAC (NR...	298572	1
Bombastus	Hydrated liniment SR/DAC (NR...	303963	2
Apomix	Hydrated liniment SR/DAC (NR...	31A040515	2
apomix/Holdermann	Hydrated liniment SR/DAC (NR...	32A120515	1
apomix/Gehe	Hydrated liniment SR/DAC (NR...	33A070514	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	33A190515	1
Bombastus	Hydrated liniment SR/DAC (NR...	4114E-03266	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	42A020614	1
apomix	Hydrated liniment SR/DAC (NR...	42A020614	1
PKH Halle / Phoenix	Hydrated liniment SR/DAC (NR...	44A220615	1
Apomix / Phönix	Hydrated liniment SR/DAC (NR...	47B170614	1
Raben-Apotheke Mildena	Hydrated liniment SR/DAC (NR...	49A230614	1
apomix	Hydrated liniment SR/DAC (NR...	60A150816	1
Apomix	Hydrated liniment SR/DAC (NR...	61A110814	1
apomix	Hydrated liniment SR/DAC (NR...	61A010915	1
aopmix/Phoenix	Hydrated liniment SR/DAC (NR...	62A110814	1
apomix	Hydrated liniment SR/DAC (NR...	62A110814	1
Raben-Apotheke Mildena	Hydrated liniment SR/DAC (NR...	63A120814	2
Apomix/Sana	Hydrated liniment SR/DAC (NR...	66A210915	1
apomix	Hydrated liniment SR/DAC (NR...	66A210915	1
Apomix	Hydrated liniment SR/DAC (NR...	67A010914	1
apomix	Hydrated liniment SR/DAC (NR...	67A010914	1
apomix PKH GmbH Halle	Hydrated liniment SR/DAC (NR...	71A051015	2
Apomix	Hydrated liniment SR/DAC (NR...	72A220914	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	75A131113	1
apomix/Holdermann	Hydrated liniment SR/DAC (NR...	76A031115	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	78A161115	1
Apomix PKH GmbH	Hydrated liniment SR/DAC (NR...	79011215	1
apomix/Gehe	Hydrated liniment SR/DAC (NR...	81A251114	1
AMH Niemann/Noweda	Hydrated liniment SR/DAC (NR...	83A021214	1
Apomix/Noweda	Hydrated liniment SR/DAC (NR...	85A091214	1
Apomix/Gehe	Hydrated liniment SR/DAC (NR...	86A161214	1
Bombastus	Hydrated liniment SR/DAC (NR...	88A161214	1
Bombastus	Hydrated liniment SR/DAC (NR...	264186	1
Bombastus	Hydrated liniment SR/DAC (NR...	269132	1
Bombastus	Hydrated liniment SR/DAC (NR...	268576	1
Phönix	Hydrated liniment SR/DAC (NR...	271895	1
Phönix Gotha	Liniment, non-ionic hydrated...	270008	1
Bombastus	Liniment, non-ionic hydrated...	272611	1
Gehe/Apomix/06.11.2013	Hydrated liniment SR/DAC (NR...	21013	1
ApoMix	Hydrated liniment SR/DAC (NR...	4A110112	1
Apomix	Hydrated liniment SR/DAC (NR...	5A210110	1
Phoenix (PKH Halle)	Hydrated liniment SR/DAC (NR...	5A210113	1
Pharmachem/Anzag/10.07...	Hydrated liniment SR/DAC (NR...	60513	1
Pharmachem/Phönix	Hydrated liniment SR/DAC (NR...	50612	1
apomix	Hydrated liniment SR/DAC (NR...	6A180112	1
Phoenix (PKH Halle)	Hydrated liniment SR/DAC (NR...	7A290113	1

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Supplier	Substance	Batch	Spectra
GEHE/Pharmachem/20.04.2...	Hydrated liniment SR/DAC (NR...	91211	1
Apomix	Hydrated liniment SR/DAC (NR...	21A180313	2
ApoMix	Hydrated liniment SR/DAC (NR...	12A150212	1
apomix 004	Hydrated liniment SR/DAC (NR...	23A270312	1
Gehe/Pharmachem /13.06....	Hydrated liniment SR/DAC (NR...	250412	1
Apomix/Phönix	Hydrated liniment SR/DAC (NR...	25A220413	1
Bombastus	Liniment, non-ionic hydrated...	269848	1
Bombastus	Hydrated liniment SR/DAC (NR...	277778	1
Bombastus	Hydrated liniment SR/DAC (NR...	277782	1
Bombastus	Hydrated liniment SR/DAC (NR...	278256	1
Caelo	Hydrated liniment SR/DAC (NR...	279398	1
Bombastus	Hydrated liniment SR/DAC (NR...	279397	1
Bombastus	Hydrated liniment SR/DAC (NR...	282882	1
Apomix	Hydrated liniment SR/DAC (NR...	33A210513	2
Apomix	Hydrated liniment SR/DAC (NR...	35A290512	1
Apomix	Hydrated liniment SR/DAC (NR...	44A120612	1
apomix	Hydrated liniment SR/DAC (NR...	48A020712	1
Apomix	Hydrated liniment SR/DAC (NR...	56A120813	1
Apomix	Hydrated liniment SR/DAC (NR...	48A170713	1
Apomix	Hydrated liniment SR/DAC (NR...	58A010812	1
apomix	Hydrated liniment SR/DAC (NR...	56A240712	1
apomix	Hydrated liniment SR/DAC (NR...	60A020812	1
Phönix (PKH Halle)	Hydrated liniment SR/DAC (NR...	60A020812	1
Caelo	Hydrated liniment SR/DAC (NR...	67b40912	1
apomix	Hydrated liniment SR/DAC (NR...	69A120912	1
Apomix	Hydrated liniment SR/DAC (NR...	69A120912	1
Apomix Phönix	Hydrated liniment SR/DAC (NR...	71A291013	1
Apomix	Hydrated liniment SR/DAC (NR...	72A011012	1
apomix	Hydrated liniment SR/DAC (NR...	80A061112	1

- 57 364 spectra from 330 *Apo-Ident* customers from a total of 19 582 batches from a further 327 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	640	0	33 704
Type B	0	1760	0	61 734
Type C	0	1068	9	57 256

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 % (> 99.9689 %)	100.0000 % (> 99.0625 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 99.6591 %)
Type C	100.0000 % (> 99.5964 %)	99.1643 % (> 98.8858 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30982	31939	7.61	42.21
31169	31169	0.00	46.54
31170	31170	0.00	40.80
31438	31939	4.16	38.78
31476	32090	6.10	45.09
31827	31947	2.25	44.58
31830	31947	1.58	43.64
31938	31938	0.00	41.10
31939	31939	0.00	39.55
31943	31943	0.00	45.31
31945	31945	0.00	45.35
31947	31947	0.00	45.61
32090	32090	0.00	44.19
32305	31170	5.42	38.98
32727	31947	9.70	42.28

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Macrogol 300**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31151-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Macrogol 300; Polyäthylenglykolum 300

Special notes

When selecting the *Macrogol 300* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Macrogol 300*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogol 300	13070109	31151	40	1403339
Caelo	Macrogol 300	14043802	31370	40	20140221
Caelo	Macrogol 300	16022102	32073	40	20160222

Validation samples

A total of 156 379 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 *Macrogol 300*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 180 spectra of 5 reference samples from the substance/substance group *Macrogol 300*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Macrogol 300	9375703	30152	40
Caelo	Macrogol 300	16022102	32073 [†]	20
Caelo	Macrogol 300	160221	32209	40
Caelo	Macrogol 300	161609	32212	40
Caelo	Macrogol 300	162196	32337	40

- 63 414 spectra from a total of 1472 batches from further 439 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.

- 36 spectra from 20 *Apo-Ident* customers from 25 batches from the substance/substance group *Macrogol 300*.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Macrogol 300	1323304	1
Caelo	Macrogol 300	13233304	5
Caelo	Macrogol 300	14145107	1
Caelo	Macrogol 300	14043802	2
Caelo	Macrogol 300	14183102	2
Phoenix am 13.03.14	Macrogol 300	13233304	1
Caelo	Macrogol 300	15286402	2
Euro OTC	Macrogol 300	4315A-02102	1
Anzag 10.12.2012	Macrogol 300	11170206	1
Caelo	Macrogol 300	11043206	1
Euro OTC	Macrogol 300	5214I-02102	1
Caelo	Macrogol 300	11336201	2
Caelo	Macrogol 300	12108103	1
Caelo	Macrogol 300	11336205	1
Caelo	Macrogol 300	12137805	1
Caelo	Macrogol 300	12108101	1
Caelo	Macrogol 300	12272906	1
Caelo	Macrogol 300	13070109	1
Caelo	Macrogol 300	1133624	1
Gehe	Macrogol 300	12137805	1
Caelo	Macrogol 300	11336204	1
Caelo	Macrogol 300	1307109	1
Gehe 21.06.2013	Macrogol 300	13070109	1
Caelo	Macrogol 300	12137803	1
Caelo	Macrogol 300		1
Caelo	Macrogol 300	1406212102	1
Euro OTC	Macrogol 300	2512051	1
Euro OTC	Macrogol 300	4312I-02102	1

- 58 405 spectra from 332 *Apo-Ident* customers from a total of 20 067 batches from a further 328 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 *Macrogol 300* 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 *Macrogol 300* 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	34 224
Type B	0	180	0	63 414
Type C	0	32	4	58 405

The substance/substance group *Macrogol 300* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.5965 %)	88.8889 % (> 80.5556 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31151	31151	0.00	50.66
31370	31151	4.12	46.89
32073	31151	12.80	43.00

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Macrogol 400**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30523-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Macrogol 400; Macrogolum 400; Polyäthylenglycolum 400

Special notes

When selecting the *Macrogol 400* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Macrogol 400*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogol 400	13171112	31149	40	1403644
Caelo	Macrogol 400	14009101	31367	40	20140123
Euro OTC	Macrogol 400	1510042	31814	40	20151216*
Euro OTC	Macrogol 400	1609017	32714	40	20160929*
Caelo	Macrogol 400	170137	33057	40	20170125*

Validation samples

A total of 156 379 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 *Macrogol 400*. These samples are listed above in the [calibration samples](#) section.
- 34 144 spectra from a total of 793 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 380 spectra of 10 reference samples from the substance/substance group *Macrogol 400*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Macrogol 400	10105810	30166	40
Euro OTC	Macrogol 400	1008004-02	30523	40
Caelo	Macrogol 400	12043301	30524	40
Euro OTC	Macrogol 400	1510042	31814 [†]	20
Euro OTC	Macrogol 400	1603008	32185	40
Euro OTC	Macrogol 400	1412015	32187	40
Caelo	Macrogol 400	160022	32211	40
Euro OTC	Macrogol 400	1607022	32461	40
Euro OTC	Macrogol 400	1610001	32712	40
Caelo	Macrogol 400	162941	33096	40

- 63 214 spectra from a total of 1467 batches from further 439 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.

*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.

[†]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*.

- 352 spectra from 114 *Apo-Ident* customers from 112 batches from the substance/substance group *Macrogol 400*.

Supplier	Substance	Batch	Spectra
Caelo	Macrogol 400	12152602	4
Fafron/Anzag	Macrogol 400	1014E-03059	1
Caelo	Macrogol 400	12277607	7
Caelo	Macrogol 400	12152614	3
Fagron	Macrogol 400	13/26-N21	1
Euro OTC	Macrogol 400	1304030-01	6
Euro OTC	Macrogol 400	130403001	1
Fagron	Macrogol 400	13126-N21	1
Caelo	Macrogol 400	13171107	5
Caelo	Macrogol 400	13171103	5
Caelo	Macrogol 400	13272901	5
Caelo	Macrogol 400	13171112	4
Caelo	Macrogol 400	13272904	5
Caelo	Macrogol 400	13272906	4
Alliance Health 14.04.2...	Macrogol 400	13272908	2
Caelo	Macrogol 400	13272909	3
Caelo	Macrogol 400	13272908	1
Fagron	Macrogol 400	13F06-B40-289978	1
Fagron	Macrogol 400	13F06-N11	9
Caelo	Macrogol 400	14009101	3
Caelo	Macrogol 400	14009102	3
Caelo	Macrogol 400	14009103	4
Caelo	Macrogol 400	14009107	6
Caelo	Macrogol 400	14009109	5
Caelo	Macrogol 400	14009110	4
Phönix	Macrogol 400	14009109	1
Caelo	Macrogol 400	14009113	3
Euro OTC	Macrogol 400	1402011-01	6
Caelo	Macrogol 400	140211-01	1
OTG/Phönix	Macrogol 400	1412015-01	1
Caelo	Macrogol 400	1409103	1
Euro OTC	Macrogol 400	1402011-11	1
Euro OTC	Macrogol 400	1412015-01	2
Euro OTC	Macrogol 400	1412015-02	1
Caelo	Macrogol 400	14195601	18
Caelo	Macrogol 400	14195602	8
Caelo	Macrogol 400	14195603	11
Caesar & Loretz GmbH	Macrogol 400	14195603	1
Caelo	Macrogol 400	14195605	5
Caelo	Macrogol 400	14352801	3
Caelo	Macrogol 400	14195613	1
Caelo	Macrogol 400	14352803	7
Bombastus	Macrogol 400	14352803	2
Caelo	Macrogol 400	14352804	3
Caelo	Macrogol 400	14352811	1
Caelo	Macrogol 400	14352805	2
Canea/Phönix	Macrogol 400	14352805	1
Caelo	Macrogol 400	14352813	3
Caelo	Macrogol 400	14352814	9
Fagron	Macrogol 400	14B05-B04-294688	1
Fagron	Macrogol 400	14C10-B05-300393	1
Euro OTC	Macrogol 400	1510042-01	2
Fagron	Macrogol 400	14G10-B05	1
Fagron	Macrogol 400	14G10-B05-300393	2
Caelo	Macrogol 400	15131406	2
Caelo	Macrogol 400	15131401	1

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Supplier	Substance	Batch	Spectra
Noweda	Macrogol 400	15131406	1
Hustadt-Apotheke	Macrogol 400	15131407	1
Caelo	Macrogol 400	15324001	3
Caelo	Macrogol 400	15324002	8
Hustadt-Apotheke	Macrogol 400	15324003	1
Caelo	Macrogol 400	15324004	1
Caelo	Macrogol 400	16002201	9
Caelo	Macrogol 400	15324007	1
Caelo	Macrogol 400	15324008	2
Noweda	Macrogol 400	15324008	1
Phoenix	Macrogol 400	16002203	1
Caelo	Macrogol 400	16002202	1
Caelo	Macrogol 400	16002203	1
Caelo	Macrogol 400	16128203	4
Hustadt-Apotheke	Macrogol 400	1716I-03059	1
Caelo	Macrogol 400	21092015B	1
Fagron	Macrogol 400	2314A-03059	1
Caelo	Macrogol 400	18081505	1
Caelo	Macrogol 400	2412U-03059	1
Euro OTC	Macrogol 400	1008004-02	1
Caelo	Macrogol 400	11172705	1
Caelo	Macrogol 400	11172707	1
Fagron	Macrogol 400	11/45	1
Caelo	Macrogol 400	11293302	1
Caelo	Macrogol 400	11293304	1
Caelo	Macrogol 400	11293311	1
Caelo	Macrogol 400	12043301	3
Noweda	Macrogol 400	11293312	1
Fagron	Macrogol 400	11I13-N04	1
Phönix 06.10.2012	Macrogol 400	12043306	1
Fagron	Macrogol 400	11F07-N01	1
Caelo	Macrogol 400	12043311	1
Caelo	Macrogol 400	12043312	2
Caelo/Gehe	Macrogol 400	12043311	1
Noweda	Macrogol 400	12043312	1
Euro OTC	Macrogol 400	1206030-01	2
Euro OTC	Macrogol 400	1206030-02	4
Phönix	Macrogol 400	1206030-01	1
Caelo	Macrogol 400	1213M-03059	1
Caelo	Macrogol 400	12152601	1
Anzag	Macrogol 400	12152601	1
Hustadt Apotheke	Macrogol 400	12152607	1
Caelo	Macrogol 400	12152607	1
Caelo	Macrogol 400	12152608	7
Caelo	Macrogol 400	12152611	2
Phoenix	Macrogol 400	12152611	1
Caelo	Macrogol 400	12152612	7
Caelo	Macrogol 400	12152613	4
Noweda	Macrogol 400	12152614	3
Phönix 26.04.2013	Macrogol 400	12152614	1
Noweda	Macrogol 400	1215614	1
Caelo	Macrogol 400	12277603	2
Phönix Gotha	Macrogol 400	12277607	1
Caelo	Macrogol 400	12277608	1
Fagron	Macrogol 400	12C21-N10	7
Fagron	Macrogol 400	12c21-n10	1
Gehe 25.04.2013	Macrogol 400	12293312	1
Caelo	Macrogol 400	12277611	1
Fagron	Macrogol 400	12H02-N05	5
Fagron	Macrogol 400	12H02-N05	1

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Supplier	Substance	Batch	Spectra
Caelo	Macrogol 400	13171102	8
Caelo	Macrogol 400	13171104	5
Caesar/Noweda	Macrogol 400	13171106	1
Caelo	Macrogol 400	13171106	3
Caelo	Macrogol 400	13171109	3
Caelo	Macrogol 400	131711102	1
Caelo	Macrogol 400	13171113	2
Fagron	Macrogol 400	13A25-N02	7
Hedinger	Macrogol 400	13F06-N11	1
Fagron	Macrogol 400	13I26-N21	1
Caelo	Macrogol 400	20021306	1
Caelo	Macrogol 400	38121-03059	1
Caelo	Macrogol 400	27111309	1
Caelo	Macrogol 400	20190612-1	1
Caelo	Macrogol 400	13141-03059	1
Caelo	Macrogol 400	1206030-02	2
Phönix	Macrogol 400	12152601	1

- 58 089 spectra from 332 *Apo-Ident* customers from a total of 19 982 batches from a further 328 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 *Macrogol 400* 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 *Macrogol 400* 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	34 144
Type B	0	370	10	63 214
Type C	0	336	16	58 089

The substance/substance group *Macrogol 400* 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 % (> 99.9690 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9710 %)	97.3684 % (> 96.5789 %)
Type C	100.0000 % (> 99.5963 %)	95.4545 % (> 94.6023 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31149	31149	0.00	23.86
31367	33057	8.02	20.37
31814	31814	0.00	24.82
32714	32714	0.00	22.34
33057	33057	0.00	23.03

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Macrogol 8 stereate type I**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30554-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Macrogol 8 stereate type I; Polyäthylenglycol-8-stearat

Special notes

When selecting the *Macrogol 8 stereate type I* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Macrogol 8 stereate type I*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogol 8 stere...	13077501	31165	40	1407187
Caelo	Macrogol 8 stere...	13324506	31453	40	AR-15-FG-001640-01
Caelo	Macrogol 8 stere...	162302	32701	40	20160824*

Validation samples

A total of 156 379 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 *Macrogol 8 stearate type I*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Macrogol 8 stearate type I*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Macrogol 8 stearate type I	11137510	30554	40
Caelo	Macrogol 8 stearate type I	162302	32339	40

- 63 514 spectra from a total of 1475 batches from further 439 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.

- 36 spectra from 16 *Apo-Ident* customers from 20 batches from the substance/substance group *Macrogol 8 stearate type I*.

Supplier	Substance	Batch	Spectra
Caelo	Macrogol 8 stearate type I	13324501	2

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

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Supplier	Substance	Batch	Spectra
Phönix	Macrogol 8 stearate type I	13324501	1
Caelo	Macrogol 8 stearate type I	13324504	4
Fagron	Macrogol 8 stearate type I	13H08-N04	1
Caelo	Macrogol 8 stearate type I	13324506	2
Fagron	Macrogol 8 stearate type I	14074603	3
Fagron	Macrogol 8 stearate type I	1515Q-03130	1
Fagron	Macrogol 8 stearate type I	14A17-B08-290544	1
Caelo	Macrogol 8 stearate type I	15249601	2
Caelo	Macrogol 8 stearate type I	14074603	2
Fagron	Macrogol 8 stearate type I	T32431	1
Caelo	Macrogol 8 stearate type I	15377301	2
Caelo	Macrogol 8 stearate type I	T30911	1
Noweda	Macrogol 8 stearate type I	11300607	1
Fagron	Macrogol 8 stearate type I	11K04-N06	1
Caelo	Macrogol 8 stearate type I	12125404	1
Fagron	Macrogol 8 stearate type I	12E24-N07	1
Noweda	Macrogol 8 stearate type I	12125404	1
Caelo	Macrogol 8 stearate type I	12E24-N07	1
Caelo	Macrogol 8 stearate type I	13077501	1
Caelo	Macrogol 8 stearate type I	12H23-N02	1
Caelo	Macrogol 8 stearate type I	13077505	2
Fagron	Macrogol 8 stearate type I	T30911	1
Fagron	Macrogol 8 stearate type I	1115M-03130	1
Fagron	Macrogol 8 stearate type I	14H04-B01-298920	1

- 58 405 spectra from 332 *Apo-Ident* customers from a total of 20 072 batches from a further 328 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 *Macrogol 8 stearate type I* 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 *Macrogol 8 stearate type I* 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	34 224
Type B	0	78	2	63 514
Type C	0	30	6	58 405

The substance/substance group *Macrogol 8 stearate type I* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	97.5000 % (> 93.7500 %)
Type C	100.0000 % (> 99.5965 %)	83.3333 % (> 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.

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
31165	31165	0.00	20.39
31453	31453	0.00	28.86
32701	32701	0.00	20.74

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Macrogol ointment**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30465-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Macrogol ointment; Unguentum polyäthylenglycoli

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Macrogol ointment*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogol ointment	13002502	31004	40	20130108
Caelo	Macrogol ointment	13177801	31247	40	1405327
Caelo	Macrogol ointment	14078601	31442	40	20140321
Caelo	Macrogol ointment	13177801	31486	40	20130709

Validation samples

A total of 156 379 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 *Macrogol ointment*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 220 spectra of 5 reference samples from the substance/substance group *Macrogol ointment*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Macrogol ointment	10033301	30255	40
Caelo	Macrogol ointment	12005903	30465	40
Caelo	Macrogol ointment	153838	31989	60
Caelo	Macrogol ointment	162577	32493	40
Caelo	Macrogol ointment	162578	32494	40

- 63 374 spectra from a total of 1472 batches from further 439 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.

- 96 spectra from 45 *Apo-Ident* customers from 41 batches from the substance/substance group *Macrogol ointment*.

Supplier	Substance	Batch	Spectra
Caelo	Macrogol ointment	6031507	1
Caelo	Macrogol ointment	1012A-02834	1
Caelo	Macrogol ointment	14012201	6

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Supplier	Substance	Batch	Spectra
Fagron	Macrogol ointment	12661402	1
Caelo	Macrogol ointment	14078601	9
Fagron	Macrogol ointment	14012201	1
Caelo	Macrogol ointment	13324902	1
Caelo	Macrogol ointment	12179102	4
Caesar & Loretz GmbH	Macrogol ointment	14078601	1
Caelo	Macrogol ointment	14336301	2
Caelo	Macrogol ointment	14336302	2
Caesar & Loretz GmbH	Macrogol ointment	14336301	1
Caelo	Macrogol ointment	14219801	1
Caelo	Macrogol ointment	14219802	1
Caelo	Macrogol ointment	15170701	2
Caelo	Macrogol ointment	312E-02834	1
Caelo	Macrogol ointment	6091202	1
Caelo	Macrogol ointment	15383902	2
Caelo	Macrogol ointment	16062002	1
Caelo	Macrogol ointment	3315A-02834	1
Caelo	Macrogol ointment	16062003	1
cesar&lorenz/Phönix	Macrogol ointment	11327702	1
Caelo	Macrogol ointment	4511M-02834	1
Ebert+Jacobi	Macrogol ointment	11277701	1
Caelo	Macrogol ointment	12117202	2
Caelo	Macrogol ointment	11277702	1
Großhandel	Macrogol ointment	12179101	2
Noweda	Macrogol ointment	12179102	1
Caelo	Macrogol ointment	12261402	1
Anzag/	Macrogol ointment	12261402	2
Caelo	Macrogol ointment	12353501	4
Caelo	Macrogol ointment	12261403	1
Anzag	Macrogol ointment	12261402	1
Anzag	Macrogol ointment	12353501	3
Caelo	Macrogol ointment	12353502	3
Caelo	Macrogol ointment	13002502	7
Caelo	Macrogol ointment	13002602	5
Caelo	Macrogol ointment	13177701	1
Großhandel	Macrogol ointment	13002602	1
Caelo	Macrogol ointment	13177702	3
Caelo	Macrogol ointment	13177801	4
Sanacorp	Macrogol ointment	13177801	1
Caelo	Macrogol ointment	13275302	1
Caelo	Macrogol ointment	13324901	1
Euro OTC	Macrogol ointment		1
Caelo	Macrogol ointment	19071305	1
Caelo	Macrogol ointment	22051304	1
Caelo	Macrogol ointment	29111202	1
Caelo	Macrogol ointment	10166302	1
Anzag	Macrogol ointment	12117202	1
Caelo	Macrogol ointment	13002601	1

- 58 345 spectra from 332 *Apo-Ident* customers from a total of 20 053 batches from a further 328 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 *Macrogol 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 *Macrogol 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	160	0	34 184
Type B	0	220	0	63 374
Type C	0	87	9	58 345

The substance/substance group *Macrogol 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.5964 %)	90.6250 % (> 87.5000 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31004	31247	19.89	39.34
31247	31247	0.00	43.77
31442	31247	17.91	34.43
31486	31247	10.03	38.14

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Macrogol-2-laurylether**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31731-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Macrogol-2-laurylether; Dehydol® LS 2

Special notes

When selecting the *Macrogol-2-laurylether* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Macrogol-2-laurylether*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogol-2-laury...	14054304	31731	40	1603434
Caelo	Macrogol-2-laury...	14054309	31867	40	20140225

Validation samples

A total of 156 379 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 *Macrogol-2-laurylether*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 64 spectra of 3 reference samples from the substance/substance group *Macrogol-2-laurylether*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Macrogol-2-laurylether	14054304	31731 [†]	20
Caelo	Macrogol-2-laurylether	14054309	31867 [†]	20
Caelo	Macrogol-2-laurylether	15411904	not required	24

- 63 530 spectra from a total of 1474 batches from further 439 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 *Macrogol-2-laurylether*.
- 58 441 spectra from 332 *Apo-Ident* customers from a total of 20 092 batches from a further 329 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](#),

[†]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 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 *Macrogol-2-laurylether* 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 *Macrogol-2-laurylether* 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	34 264
Type B	0	64	0	63 530
Type C	0	0	0	58 441

The substance/substance group *Macrogol-2-laurylether* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.6250 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31731	31731	0.00	25.88
31867	31731	6.95	23.39

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Mandarine peel oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31747-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Mandarine peel oil; Oleum Mandarinæ

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Mandarine peel oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Mandarine peel oil	14064103	31747	40	1602210
Caelo	Mandarine peel oil	15398001	31863	40	20151127

Validation samples

A total of 156 379 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 *Mandarine peel oil*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 92 spectra of 4 reference samples from the substance/substance group *Mandarine peel oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Mandarine peel oil	14064103	31747 [†]	20
Caelo	Mandarine peel oil	15398001	31863 [†]	20
Caelo	Mandarine peel oil	170368	33074	40
Caelo	Mandarine peel oil	15011601	not required	12

- 63 502 spectra from a total of 1473 batches from further 439 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 *Mandarine peel oil*.

Supplier	Substance	Batch	Spectra
Taoasis	Mandarine peel oil	412011-124957	1

[†]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*.

- 58 440 spectra from 332 *Apo-Ident* customers from a total of 20 091 batches from a further 328 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 *Mandarine peel 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 *Mandarine peel 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	34 264
Type B	0	92	0	63 502
Type C	0	1	0	58 440

The substance/substance group *Mandarine peel 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 93.4783 %)
Type C	100.0000 % (> 99.6053 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31747	31747	0.00	19.70
31863	31747	5.26	18.83

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Matricaria oil, rich in (-)-alpha-bisabolol
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30738-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Matricaria oil, rich in (-)-alpha-bisabolol; Oleum chamomillae

Special notes

When selecting the *Matricaria oil, rich in (-)-alpha-bisabolol* substance/substance group, the following information is displayed to the user:

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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, rich in (-)-alpha-bisabolol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Matricaria oil, ...	11221206	30738	40	20110810
Caelo	Matricaria oil, ...	13195103	31239	30	1504133
Caelo	Matricaria oil, ...	13334702	31427	40	20131009
Caelo	Matricaria oil, ...	13334702	31428	40	20131009

Validation samples

A total of 156 379 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 *Matricaria oil, rich in (-)-alpha-bisabolol*. These samples are listed above in the [calibration samples](#) section.
- 34 194 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 100 spectra of 4 reference samples from the substance/substance group *Matricaria oil, rich in (-)-alpha-bisabolol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Matricaria oil, rich in (-)-...	13195101	31160	20
Caelo	Matricaria oil, rich in (-)-...	13334702	31427 [†]	20
Caelo	Matricaria oil, rich in (-)-...	13334702	31428 [†]	20
Caelo	Matricaria oil, rich in (-)-...	163310	33081	40

- 63 494 spectra from a total of 1474 batches from further 439 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 8 batches from the substance/substance group *Matricaria oil, rich in (-)-alpha-bisabolol*.

[†]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*.

Supplier	Substance	Batch	Spectra
Taoasis	Matricaria oil, rich in (-)-...	16266-119132	1
Taoasis	Matricaria oil, rich in (-)-...	6181024-122141	1
Taoasis	Matricaria oil, rich in (-)-...	6181024-121466	1
Taoasis	Matricaria oil, rich in (-)-...	6181024-123770	1
Taoasis	Matricaria oil, rich in (-)-...	929-115334	1
Caelo	Matricaria oil, rich in (-)-...	18091401	1
Taoasis	Matricaria oil, rich in (-)-...	6181024-123496	1
Caelo	Matricaria oil, rich in (-)-...	15137801	1

- 58 433 spectra from 332 *Apo-Ident* customers from a total of 20 084 batches from a further 328 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, rich in (-)-alpha-bisabolol* 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, rich in (-)-alpha-bisabolol* 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	34 194
Type B	0	100	0	63 494
Type C	0	8	0	58 433

The substance/substance group *Matricaria oil, rich in (-)-alpha-bisabolol* 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 % (> 99.9690 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.5974 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30738	31239	13.90	42.92
31239	31239	0.00	42.05
31427	31239	6.58	41.08
31428	31239	6.76	41.14

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Melissa oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30207-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Melissa oil; Oleum melissae rectific.

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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
Caelo	Melissa oil	13086306	31163	40	1403319
Caelo	Melissa oil	13354110	31403	40	20131028
Caelo	Melissa oil	163349	33080	40	20161215*

Validation samples

A total of 156 379 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 *Melissa oil*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 50 spectra of 1 reference samples from the substance/substance group *Melissa oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Melissa oil	10019701	30207	50

- 63 544 spectra from a total of 1476 batches from further 439 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.

- 97 spectra from 43 *Apo-Ident* customers from 41 batches from the substance/substance group *Melissa oil*.

Supplier	Substance	Batch	Spectra
Caelo	Melissa oil	12283804	6
Caelo	Melissa oil	12253804	1
Caelo	Melissa oil	12283809	6

continued on the next page

*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.

continued from previous page

Supplier	Substance	Batch	Spectra
Nachprüfung	Melissa oil	130863060	1
Caelo	Melissa oil	13086308	5
Caelo	Melissa oil	14332501	5
Caelo	Melissa oil	13354113	2
Sanacorp	Melissa oil	1334110	1
Caelo	Melissa oil	14332511	7
Caelo	Melissa oil	13354110	2
Caelo	Melissa oil	15172303	7
Caelo	Melissa oil	11035803	1
Caelo	Melissa oil	15172308	4
Caelo	Melissa oil	18081501	1
Caelo	Melissa oil	11323902	3
Caesar&lorenz,Anzag	Melissa oil	11323902	1
Caesar & Loretz GmbH, 4...	Melissa oil	11323910	1
Anzag 27.02.13 ek: 8.17EUR	Melissa oil	122833801	1
Caelo	Melissa oil	122283804	1
Caelo	Melissa oil	11323911	1
Caelo	Melissa oil	11323903	1
Caelo	Melissa oil	12283801	2
DEFEKTUR	Melissa oil	12283809	2
celo/phönix	Melissa oil	12283805	1
Caelo	Melissa oil	12283805	1
Phönix	Melissa oil	12283809	1
Caelo	Melissa oil	13086306	3
Sanacorp	Melissa oil	13086306	1
Caelo	Melissa oil	13086311	5
Caelo	Melissa oil	14332508	2
Caelo	Melissa oil	20230712-7	1
Caelo	Melissa oil	21111303	1
Caelo	Melissa oil	5211R-01993	1
Caelo	Melissa oil	17012014	1
Caelo	Melissa oil	Ch12283804	1
Caelo	Melissa oil	28051311	1
Caelo	Melissa oil	17091201	1
Caelo	Melissa oil	13354105	2
Caelo	Melissa oil	13086310	3
Caelo	Melissa oil	13354108	1
Caelo	Melissa oil	14332504	2
Caelo	Melissa oil	14332512	1
Caelo	Melissa oil	15172310	1
Caelo	Melissa oil	13086304	1
Caelo	Melissa oil	4110I-01993	1
Caelo	Melissa oil	11323909	2

- 58 344 spectra from 332 *Apo-Ident* customers from a total of 20 052 batches from a further 328 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	120	0	34 224
Type B	0	50	0	63 544
Type C	0	96	1	58 344

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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 88.0000 %)
Type C	100.0000 % (> 99.5964 %)	98.9691 % (> 95.8763 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31163	31163	0.00	46.66
31403	31163	4.84	44.49
33080	33080	0.00	48.13

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Methyl salicylate**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31038-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Methyl salicylate; Methylis salicylas; Methylum salicylicum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Methyl salicylate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Methyl salicylate	12215217	31038	40	1403162
Fagron	Methyl salicylate	14D03-B04-294169	31607	40	20140414

Validation samples

A total of 156 379 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 *Methyl salicylate*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 61 spectra of 2 reference samples from the substance/substance group *Methyl salicylate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Methyl salicylate	10179004	30330	41
Fagron	Methyl salicylate	14D03-B04-294169	31607 [†]	20

- 63 533 spectra from a total of 1475 batches from further 439 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.

- 57 spectra from 28 *Apo-Ident* customers from 34 batches from the substance/substance group *Methyl salicylate*.

Supplier	Substance	Batch	Spectra
Caelo	Methyl salicylate	13185101	3
Bomb/ Noweda	Methyl salicylate	RMS1332311	1
Caelo	Methyl salicylate	12215215	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
Caelo	Methyl salicylate	12308307	1
Fagron	Methyl salicylate	15809-B04	1
Caelo	Methyl salicylate	13189309	2
Fagron	Methyl salicylate	13I11-N06	1
Fagron	Methyl salicylate	15H04-B01	1
Fagron	Methyl salicylate	15B09-B04	1
Caelo	Methyl salicylate	15117910	1
Caelo	Methyl salicylate	10313708	3
Fagron	Methyl salicylate	11H30-N14	1
Nachprüfung	Methyl salicylate	12D27-N05	2
Caelo	Methyl salicylate	13189308	1
Alliance Health 18.11.2...	Methyl salicylate	13185102	1
Fagron	Methyl salicylate	14D03-B04	1
PHOENIX 08.05.2014	Methyl salicylate	13I11-N06	1
Fagron	Methyl salicylate	14D03-B04-292643	1
Fagron	Methyl salicylate	14D03-B04-294169	1
Caelo	Methyl salicylate	14D03-B04-294169	1
Caelo	Methyl salicylate	15117904	1
Caelo	Methyl salicylate	15B09-B04	1
Fagron	Methyl salicylate	15B09-B04303941	1
Fagron	Methyl salicylate	RMS1332311	1
Caelo	Methyl salicylate	7111203	1
Alliance Health 10.06.2...	Methyl salicylate	RMS1332311	1
Fagron	Methyl salicylate	30121414	1
Fagron	Methyl salicylate	RMS13332311	1
Fagron	Methyl salicylate	711Q-01867	1
Fagron	Methyl salicylate	11D08-N07	3
Caesar & Loretz GmbH, 4...	Methyl salicylate	12215215	1
Fagron	Methyl salicylate	12D24-N09	1
Fagron	Methyl salicylate	12C02-No2	1
Fagron	Methyl salicylate	12D27-N05	3
Fagron	Methyl salicylate	12D27-n05	1
Fagron	Methyl salicylate	13D24-N09	3
Fagron	Methyl salicylate	13/11-N06	2
Phönix	Methyl salicylate	13D24-N09	1
Fagron	Methyl salicylate	13d24-no9	1
Fagron	Methyl salicylate	172650-0002	2
Fagron	Methyl salicylate	19061309	1
Caelo	Methyl salicylate	13I11-N06	1
Caelo	Methyl salicylate	90328419	1

- 58 384 spectra from 332 *Apo-Ident* customers from a total of 20 059 batches from a further 328 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 *Methyl salicylate* 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 *Methyl salicylate* 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	34 264
Type B	0	61	0	63 533
Type C	0	57	0	58 384

The substance/substance group *Methyl salicylate* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.1639 %)
Type C	100.0000 % (> 99.5964 %)	100.0000 % (> 89.4737 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31038	31038	0.00	154.65
31607	31038	6.77	155.42

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Metronidazole 25% in white petrolatum**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30663-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Metronidazole 25% in white petrolatum

Special notes

When selecting the *Metronidazole 25% in white petrolatum* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Metronidazole 25% in white petrolatum*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metronidazole 25...	12266401	30663	19	1405100
Caelo	Metronidazole 25...	14116801	31316	20	20140411
Caelo	Metronidazole 25...	16063101	32456	40	20160229
Caelo	Metronidazole 25...	16063101	32768	40	20160229

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 119 spectra of 4 reference samples from the substance/substance group *Metronidazole 25% in white petrolatum*. These samples are listed above in the [calibration samples](#) section.
- 34 225 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 3 reference samples from the substance/substance group *Metronidazole 25% in white petrolatum*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Metronidazole 25% in white p...	11214101	30420	40
Caelo	Metronidazole 25% in white p...	12266401	30663 [†]	20
Caelo	Metronidazole 25% in white p...	14116801	31316 [†]	20

- 63 514 spectra from a total of 1474 batches from further 439 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 9 *Apo-Ident* customers from 12 batches from the substance/substance group *Metronidazole 25% in white petrolatum*.

Supplier	Substance	Batch	Spectra
Caelo	Metronidazole 25% in white p...	14116801	3

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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
Noweda 20.02.2015	Metronidazole 25% in white p...	14247301	1
celo/Jenne	Metronidazole 25% in white p...	13077601	1
Caelo	Metronidazole 25% in white p...	16063101	2
Caelo	Metronidazole 25% in white p...	15207101	1
Caelo	Metronidazole 25% in white p...	13109801	3
Caelo	Metronidazole 25% in white p...	13188901	1
Caelo	Metronidazole 25% in white p...	13296501	2
Caelo	Metronidazole 25% in white p...	14024301	2
GEHE/26.02.2013	Metronidazole 25% in white p...	12306601	1
Caelo	Metronidazole 25% in white p...	1285301	1
Caelo	Metronidazole 25% in white p...	13077601	2
Caelo	Metronidazole 25% in white p...	13002801	2

- 58 419 spectra from 332 *Apo-Ident* customers from a total of 20 080 batches from a further 328 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 *Metronidazole 25% in white petrolatum* 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 *Metronidazole 25% in white petrolatum* 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	119	0	34 225
Type B	0	60	20	63 514
Type C	0	21	1	58 419

The substance/substance group *Metronidazole 25% in white petrolatum* 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 % (> 99.9691 %)	100.0000 % (> 94.9580 %)
Type B	100.0000 % (> 99.9711 %)	75.0000 % (> 71.2500 %)
Type C	100.0000 % (> 99.5967 %)	95.4545 % (> 81.8182 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30663	30663	0.00	46.84
31316	30663	6.87	46.09
32456	30663	16.31	47.76
32768	30663	23.48	48.34

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Mint oil / Peppermint oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30856-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mint oil / Peppermint oil; Menthae arvensis aetheroleum partim mentholum depletum; Menthae piperitae aetheroleum; Mint oil; Oleum Menthae arvens. var. piper. japanisch; Oleum menthae arvensis; Oleum menthae piperitae dopp. rectific.; Peppermint oil

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Mint oil / Peppermint oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Peppermint oil	12114206	30856	40	20120424
Euro OTC	Peppermint oil	1312009-01	31294	40	20140130

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Peppermint oil	13303915	31410	40	1502136
Euro OTC	Peppermint oil	1512011	31811	40	20151214*
Caelo	Mint oil	16053503	32474	40	1701393
Caelo	Mint oil	15380507	32476	40	1701394
Caelo	Mint oil	16053503	32780	40	20160309
Caelo	Mint oil	15380509	32781	40	20151116

Validation samples

A total of 156 379 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 *Mint oil / Peppermint oil*. These samples are listed above in the [calibration samples](#) section.
- 34 024 spectra from a total of 791 batches from further 223 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 180 spectra of 5 reference samples from the substance/substance group *Mint oil / Peppermint oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Peppermint oil	1512011	31811 [†]	20
Caelo	Peppermint oil	161904	32333	40
Euro OTC	Peppermint oil	1607018	32468	40
Caelo	Mint oil	15380507	32484	40
Caelo	Mint oil	16053508	32845	40

- 63 414 spectra from a total of 1472 batches from further 438 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the

*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.

[†]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*.

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.

- 359 spectra from 159 *Apo-Ident* customers from 150 batches from the substance/substance group *Mint oil / Peppermint oil*.

Supplier	Substance	Batch	Spectra
Fagron	Peppermint oil	13/04-N10	2
Fagron	Peppermint oil	13I04-N01	6
Fagron	Peppermint oil	14B03-B40-295665	2
Bombastus	Peppermint oil	14150216	1
Bombastus	Peppermint oil	285715	1
Bombastus	Peppermint oil	287325	1
Bombastus	Peppermint oil	286376	1
Fagron	Peppermint oil	13I04-N10	4
Bombastus	Peppermint oil	290301	4
Fagron	Peppermint oil	12D10-N04	6
Bombastus	Peppermint oil	289675	1
Fagron	Peppermint oil	700599	1
Bombastus	Peppermint oil	287528	3
Fagron	Peppermint oil	13A10-N08	4
Bombastus	Peppermint oil	279930	4
Caelo	Peppermint oil	13303915	10
Caelo	Peppermint oil	13318004	1
Caelo	Peppermint oil	14150214	7
Caelo	Peppermint oil	14150221	3
Caelo	Peppermint oil	14369909	6
Caelo	Peppermint oil	15255801	11
Caelo	Peppermint oil	15255811	5
Fagron	Peppermint oil	15B11-B08-308854	1
Caelo	Peppermint oil	16114602	1
Bombastus	Peppermint oil	288864	2
Bombastus	Peppermint oil	292138	2
Bombastus	Peppermint oil	294293	2
Bombastus	Peppermint oil	295599	2
Caelo	Peppermint oil	298969	1
Bombastus	Peppermint oil	299058	1
Caelo	Peppermint oil	11124706	1
Anzag	Peppermint oil	11G19N07	1
Fagron	Peppermint oil	11g19-n07	1
Fiebig	Peppermint oil	21022172/1	1
Bombastus	Peppermint oil	274804	1
Bombastus	Peppermint oil	275481	3
Bombastus	Peppermint oil	278812	1
Bombastus	Peppermint oil	280894	1
Bombastus	Peppermint oil	284588	1
Bombastus	Peppermint oil	286204	3
Caelo	Peppermint oil	11287407	6
Caelo	Peppermint oil	13/04-N01	1
Fagron	Peppermint oil	1304-N01	1
Caelo	Peppermint oil	13105801	5
Hedinger/Gehe	Peppermint oil	13105801	1
Gehe	Peppermint oil	13105801	1
Caelo	Peppermint oil	13241303	8

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Supplier	Substance	Batch	Spectra
Caelo	Peppermint oil	13303903	4
Caelo	Peppermint oil	13303904	5
Caelo	Peppermint oil	13303912	2
Caelo	Peppermint oil	13303914	1
Sanacorp	Peppermint oil	13303915	3
Phönix	Peppermint oil	13303915	1
Taoasis	Peppermint oil	13486-116309	1
Fagron	Peppermint oil	13104-N10	1
Euro OTC	Peppermint oil	1410005-01	1
Caeo	Peppermint oil	14150209	1
Caelo	Peppermint oil	14150209	5
sanacorp	Peppermint oil	14150214	1
Caelo	Peppermint oil	14150218	1
Caelo	Peppermint oil	14150215	1
Caelo	Peppermint oil	14150220	4
Caelo	Peppermint oil	14150225	5
Phönix Gotha	Peppermint oil	14150225	1
Caelo	Peppermint oil	14369910	1
Caelo	Peppermint oil	14369911	2
Fagron	Peppermint oil	14B03B40	1
Fagron	Peppermint oil	14B03-B40	3
Euro OTC	Peppermint oil	1512011-01	1
Euro OTC	Peppermint oil	1504017-01	1
Caelo	Peppermint oil	15126904	1
Caelo	Peppermint oil	15127004	3
Caelo	Peppermint oil	15255816	1
Euro OTC	Peppermint oil	15255816	1
Caelo	Peppermint oil	15255817	1
Caelo	Peppermint oil	15363201	2
Fagron	Peppermint oil	15B11-B08	1
Fagron	Peppermint oil	15B11-B08-304117	1
Fagron	Peppermint oil	15K27-B01-317773	1
Fagron	Peppermint oil	16F01-B03-322190	1
Alliance Healthcare	Peppermint oil	16F01-B03-322190	1
Fagron	Peppermint oil	16F01-B03-322818	1
Caelo	Peppermint oil	20111417	1
GEHE 06.06.2014	Peppermint oil	283491	1
Bombastus	Peppermint oil	283491	3
Bombastus	Peppermint oil	283734	1
Fagron	Peppermint oil	285571	1
Bombastus	Peppermint oil	285571	1
Bombastus	Peppermint oil	290394	1
Bombastus	Peppermint oil	292472	3
Bombastus	Peppermint oil	294802	1
Bombastus	Peppermint oil	295985	2
Bombastus	Peppermint oil	297256	1
Taoasis	Peppermint oil	31145-118741	1
Taoasis	Peppermint oil	37979-120290	1
Caelo	Peppermint oil	3913I-01995	1
Caelo	Peppermint oil	4214U-01995	1
Taoasis	Peppermint oil	6316-115825	1
Bio-Diät / Phönix	Peppermint oil	20553	1
Caelo	Peppermint oil	10235317	1
Bombastus	Peppermint oil	1001311995	1
Caelo	Peppermint oil	11071312	1
Caelo	Peppermint oil	11124709	3
Euro OTC	Peppermint oil	110800801	1
Caelo	Peppermint oil	11124710	3
Noweda	Peppermint oil	11124710	1
Phönix	Peppermint oil	11124710	1

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Supplier	Substance	Batch	Spectra
Caelo	Peppermint oil	11287416	8
Sanacorp	Peppermint oil	11287416	1
Caelo	Peppermint oil	11287419	1
Caelo	Peppermint oil	11287421	5
Fagron	Peppermint oil	11A05-N02	1
Fagron	Peppermint oil	11C14-N06	1
Fagron	Peppermint oil	11G19-N07	3
Fagron	Peppermint oil	11F09-N12	1
Caelo	Peppermint oil	12020803	1
Fagron	Peppermint oil	12/19-N09	1
Caelo	Peppermint oil	12020812	1
Caelo	Peppermint oil	12020815	1
Caelo	Peppermint oil	12114206	15
Fagron	Peppermint oil	12114206	1
Hedinger	Peppermint oil	12114206	1
Noweda	Peppermint oil	12114206	1
Sanacorp	Peppermint oil	12114206	1
Caelo	Peppermint oil	12114211	1
Phoenix	Peppermint oil	12114211	1
Caelo	Peppermint oil	12114219	4
Sanacorp	Peppermint oil	12114219	1
Caelo	Peppermint oil	12114224	2
Caelo	Peppermint oil	12114225	14
Caesar & Loretz GmbH, 4...	Peppermint oil	12184601	2
Euro OTC	Peppermint oil	1303015-01	2
Caelo	Peppermint oil	13105306	1
Caelo	Peppermint oil	13105905	3
Caelo	Peppermint oil	13241306	1
Caelo	Peppermint oil	1324302	1
Gehe	Peppermint oil	13303903	1
Caesar/Noweda	Peppermint oil	13303915	1
Caelo	Peppermint oil	13318201	1
Fagron	Peppermint oil	13A10N08	2
Caelo	Peppermint oil	13A10-N08	2
Fagron	Peppermint oil	13A10-N8	1
Fagron	Peppermint oil	13i04-N10	1
Caelo	Peppermint oil	20151112-6	1
Caelo	Peppermint oil	2112E-01995	1
Fagron	Peppermint oil	250214PJK02	1
Fagron	Peppermint oil	267849	1
Bombastus	Peppermint oil	269560	1
Caelo	Peppermint oil	269560	1
Anzag ek:13.70EUR 15.08.12	Peppermint oil	270566	1
Bombastus	Peppermint oil	271257	1
Phönix 10.01.13	Peppermint oil	273025	1
Bombastus	Peppermint oil	277504	4
DEFEKTUR	Peppermint oil	277504	1
Bombastus	Peppermint oil	277817	2
Sanacorp	Peppermint oil	280894	1
AHD, 29.11.13	Peppermint oil	282542	1
Phönix	Peppermint oil	287529	1
Bombastus	Peppermint oil	295737	1
phönix	Peppermint oil		1
Caelo	Peppermint oil	46/AD1	1
Sanacorp	Peppermint oil	47/AKD19	1
Taoasis	Peppermint oil	515574-107811	1
Taoasis	Peppermint oil	512777-107965	1
Taoasis	Peppermint oil	501319-105273	1
Taoasis	Peppermint oil	525728-109630	1
Taoasis	Peppermint oil	539490-111157	2

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Supplier	Substance	Batch	Spectra
Taoasis GmbH	Peppermint oil	534640-110874	1
Taoasis	Peppermint oil	548992-112346	3
Caelo	Peppermint oil	688901	2
Fagron	Peppermint oil	688901	1
Bombastus	Peppermint oil	80312004	1
Fagron	Peppermint oil	8574769	2
	Peppermint oil	9183299	1
Sensient	Peppermint oil	C9982	1
Taomed	Peppermint oil		1
Caelo	Peppermint oil	Ch12114219	1
Bombastus	Peppermint oil		1

- 58 082 spectra from 332 *Apo-Ident* customers from a total of 19 944 batches from a further 328 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 *Mint oil / 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 *Mint oil / 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	320	0	34 024
Type B	0	180	0	63 414
Type C	0	324	35	58 082

The substance/substance group *Mint oil / 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 % (> 99.9689 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.5963 %)	90.2507 % (> 89.4150 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30856	31410	11.46	52.72
31294	31811	2.57	55.84
31410	31410	0.00	55.05
31811	31811	0.00	55.61
32474	32474	0.00	59.84
32476	32476	0.00	54.55
32780	32474	3.85	59.81
32781	32476	5.34	55.69

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Mountain pine oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30204-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mountain pine oil; Oleum pini pumilionis; Pini pumilionis aetherolum

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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 *Mountain pine oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Mountain pine oil	12C29-N17	31184	40	1403167
Caelo	Mountain pine oil	11375614	31189	40	20120102
Euro OTC	Mountain pine oil	1210024-02	31529	40	20140806
Euro OTC	Mountain pine oil	1511014	31818	40	20151214*
Caelo	Mountain pine oil	16114705	33266	40	20160420

Validation samples

A total of 156379 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 *Mountain pine oil*. These samples are listed above in the [calibration samples](#) section.
- 34144 spectra from a total of 793 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 160 spectra of 5 reference samples from the substance/substance group *Mountain pine oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Mountain pine oil	10060307	30204	40
Euro OTC	Mountain pine oil	1210024-02	31529 [†]	20
Euro OTC	Mountain pine oil	1511014	31818 [†]	20
Euro OTC	Mountain pine oil	1606003	32470	40
Euro OTC	Mountain pine oil	1703031	33235	40

- 63434 spectra from a total of 1472 batches from further 439 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.

*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.

[†]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*.

- 106 spectra from 58 *Apo-Ident* customers from 54 batches from the substance/substance group *Mountain pine oil*.

Supplier	Substance	Batch	Spectra
Phönix	Mountain pine oil	11/19-N12	1
Caelo	Mountain pine oil	11375614	3
Frey+Lau GmbH/Phönix	Mountain pine oil	12C29-N17	2
Euro OTC	Mountain pine oil	1210024-02	1
Fagron	Mountain pine oil	12-K06-N06	1
Fagron	Mountain pine oil	12K06-N06	1
Fagron	Mountain pine oil	13C04-N02	5
Fagron	Mountain pine oil	13E06-N04	3
Frey & Lau GmbH/Phoenix	Mountain pine oil	13C04-N020133/265	1
Caelo	Mountain pine oil	14083301	3
Caelo	Mountain pine oil	14083302	3
Caelo	Mountain pine oil	14083311	1
Caelo	Mountain pine oil	14083303	1
Euro OTC	Mountain pine oil	1411021-01	5
Caelo	Mountain pine oil	14083315	1
Caelo	Mountain pine oil	15239202	2
Fagron	Mountain pine oil	15051509	1
Euro OTC	Mountain pine oil	1511014-01	2
Fagron	Mountain pine oil	15A05-B06-305065	1
Caelo	Mountain pine oil	21051403	1
Taoasis	Mountain pine oil	25599-117839	1
Taoasis	Mountain pine oil	25599-118829	1
Fritz Schiele	Mountain pine oil		1
Taoasis	Mountain pine oil	586/116867	1
Taoasis	Mountain pine oil	586-116867	1
Fagron	Mountain pine oil	736339	3
Taoasis	Mountain pine oil	8783-125163	1
Caelo	Mountain pine oil	10020505	1
Caelo	Mountain pine oil	1792977	2
Caelo	Mountain pine oil	11069807	1
Caelo	Mountain pine oil	11357601	1
Caelo	Mountain pine oil	11375601	11
Klenk	Mountain pine oil	11375601	1
Alliance	Mountain pine oil	11375601	1
Caelo	Mountain pine oil	11375608	1
Caelo	Mountain pine oil	11375613	3
Fagron	Mountain pine oil	11G18-N10	2
Fagron	Mountain pine oil	11L19-N12	1
Caelo	Mountain pine oil	12239902	2
Caelo	Mountain pine oil	12239904	2
Caelo	Mountain pine oil	12239903	1
Fagron	Mountain pine oil	12C29-N17	2
Fagron	Mountain pine oil	12G12-N11	2
PVL	Mountain pine oil	1360313	1
Fargo	Mountain pine oil	13C04-N02	1
Fagron	Mountain pine oil	13C04-N02	1
Caelo	Mountain pine oil	17012014	2
Fagron	Mountain pine oil	27111207	1
Caelo	Mountain pine oil	23021301	1
Taoasis GmbH	Mountain pine oil	30985-110461	1
Taoasis	Mountain pine oil	30985-111105	2
Taoasis	Mountain pine oil	33347-112503	1
Taoasis	Mountain pine oil	30985-110461	1
Fagron	Mountain pine oil	14D14-B01	5
Fagron	Mountain pine oil	15A05-B06	3
Caelo	Mountain pine oil	16114701	1
Caelo	Mountain pine oil	1137575601	1

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Supplier	Substance	Batch	Spectra
Taoasis	Mountain pine oil	30985-106654	1
Fagron	Mountain pine oil	13H28-N04	1

- 58 335 spectra from 332 *Apo-Ident* customers from a total of 20 040 batches from a further 328 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 *Mountain 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 *Mountain 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	200	0	34 144
Type B	0	159	1	63 434
Type C	0	96	10	58 335

The substance/substance group *Mountain 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 % (> 99.9690 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9710 %)	99.3750 % (> 97.5000 %)
Type C	100.0000 % (> 99.5964 %)	90.5660 % (> 87.7358 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31184	31184	0.00	40.64
31189	31184	4.15	41.80

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31529	31818	2.11	42.84
31818	31818	0.00	40.80
33266	31818	6.14	44.03

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Myrtle oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31836-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Myrtle oil; Oleum myrte

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Myrtle oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Myrtle oil	15225102	31836	40	1606483
Caelo	Myrtle oil	15225102	32349	40	20150721

Validation samples

A total of 156 379 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 *Myrtle oil*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 797 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Myrtle oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Myrtle oil	15225102	31836 [†]	20
Caelo	Myrtle oil	15225103	32182	40

- 63 534 spectra from a total of 1475 batches from further 439 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 *Myrtle oil*.
- 58 441 spectra from 332 *Apo-Ident* customers from a total of 20 092 batches from a further 329 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](#).

[†]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*.

Validation results

The validation runs checked whether the substance/substance group *Myrtle 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 *Myrtle 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	34 264
Type B	0	60	0	63 534
Type C	0	0	0	58 441

The substance/substance group *Myrtle 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31836	31836	0.00	27.27
32349	31836	3.42	29.10

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Octyldodecanol**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30867-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Octyldodecanol; Octyldodecanolum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Octyldodecanol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Octyldodecanol	12165509	30867	40	20120711
Caelo	Octyldodecanol	13360010	31330	40	AR-15-FG-000314-01
Caelo	Octyldodecanol	15135212	31753	40	20150506
Caelo	Octyldodecanol	16095507	32958	40	20160421

Validation samples

A total of 156 379 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 *Octyldodecanol*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 96 spectra of 4 reference samples from the substance/substance group *Octyldodecanol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Octyldodecanol	15135212	31753 [†]	20
Caelo	Octyldodecanol	163127	33093	40
Caelo	Octyldodecanol	16095506	not required	24
Fagron	Octyldodecanol	16G20-B99-324356	not required	12

- 63 498 spectra from a total of 1473 batches from further 439 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.

- 738 spectra from 194 *Apo-Ident* customers from 131 batches from the substance/substance group *Octyldodecanol*.

Supplier	Substance	Batch	Spectra
Caelo	Octyldodecanol	14371706	10

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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
Caelo	Octyldodecanol	13360010	14
Phoenix	Octyldodecanol	13360006	1
Caelo	Octyldodecanol	14371711	17
Caelo	Octyldodecanol	13222011	3
Caelo	Octyldodecanol	13360011	13
Caelo	Octyldodecanol	14130205	8
Caelo	Octyldodecanol	13360008	11
Caelo	Octyldodecanol	14158410	7
Caelo	Octyldodecanol	2613M-02875	2
Caelo	Octyldodecanol	14130207	25
Caelo	Octyldodecanol	3314E-02875	1
Caelo	Octyldodecanol	10281907	1
Caelo	Octyldodecanol	11060319	3
Gehe	Octyldodecanol	11060308	1
Caelo	Octyldodecanol	1136017	1
Caelo	Octyldodecanol	11060312	1
Caelo	Octyldodecanol	11369003	8
Caelo	Octyldodecanol	11369004	3
Caelo	Octyldodecanol	11369012	2
Caelo	Octyldodecanol	11369014	2
Caelo	Octyldodecanol	11369016	7
Gehe	Octyldodecanol	11369012	1
phönix, 20.11.2012	Octyldodecanol	11369017	2
Caelo	Octyldodecanol	11369021	6
Caelo	Octyldodecanol	11369017	6
Gehe	Octyldodecanol	11369021	1
Caelo	Octyldodecanol	12091304	1
Caelo	Octyldodecanol	12165506	4
Gehe	Octyldodecanol	12165506	1
Caelo	Octyldodecanol	12165509	4
Caelo	Octyldodecanol	12165511	11
Noweda	Octyldodecanol	11369021	1
phönix, 05.12.2012	Octyldodecanol	12165511	1
Anzag	Octyldodecanol	12165509	1
Caelo	Octyldodecanol	12165515	8
Caelo	Octyldodecanol	12165514	4
Noweda	Octyldodecanol	12165515	1
Anzag, 20.03.2013	Octyldodecanol	12165515	2
Gehe	Octyldodecanol	12165515	2
Caelo	Octyldodecanol	12165519	9
Caelo	Octyldodecanol	12165517	2
Gehe	Octyldodecanol	12165519	1
Caelo	Octyldodecanol	12165520	10
Phönix	Octyldodecanol	12165521	3
Caelo	Octyldodecanol	12165521	11
Phönix	Octyldodecanol	13044005	1
Caelo	Octyldodecanol	13044002	9
Caelo	Octyldodecanol	13044013	19
Alliance healthcare	Octyldodecanol	13044013	1
Beiersdorf/Anzag	Octyldodecanol	13044007	1
Caelo	Octyldodecanol	13044010	10
Caelo	Octyldodecanol	13222003	18
Caelo	Octyldodecanol	13044015	5
Caelo	Octyldodecanol	13044016	18
Phönix	Octyldodecanol	13222008	1
Caelo	Octyldodecanol	13222008	16
Caelo	Octyldodecanol	15135203	7
Caelo	Octyldodecanol	15383004	7
Caelo	Octyldodecanol	82695089	1
Caelo	Octyldodecanol		2

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Supplier	Substance	Batch	Spectra
Caelo	Octyldodecanol	15135211	8
Caelo	Octyldodecanol	26071208	1
Caelo	Octyldodecanol	B11060317	1
Caelo	Octyldodecanol	13360002	13
Fagron	Octyldodecanol	200714112-2	1
Caelo	Octyldodecanol	516A-02875	1
Nachprüfung	Octyldodecanol	13044015	2
Caelo	Octyldodecanol	1314I-02875	1
Caelo	Octyldodecanol	13222002	9
Caelo	Octyldodecanol	133360010	1
Caelo	Octyldodecanol	13222013	1
Caelo	Octyldodecanol	13360001	3
Caelo	Octyldodecanol	13360003	7
Noweda	Octyldodecanol	13360003	1
Caesar & Loretz	Octyldodecanol	13360003	1
Caelo	Octyldodecanol	13360005	4
Caelo	Octyldodecanol	13360006	12
Caesar & Loretz GmbH	Octyldodecanol	13360010	1
Caelo	Octyldodecanol	13360009	1
PHOENIX 30.06.2014	Octyldodecanol	13360011	1
Caelo	Octyldodecanol	13360012	9
Noweda	Octyldodecanol	13360012	1
Fagron	Octyldodecanol	13L02-B05	2
Sanacorp	Octyldodecanol	13102-b05-288974	1
Caelo	Octyldodecanol	14130204	1
Caelo	Octyldodecanol	14130202	1
Caelo	Octyldodecanol	14130205	1
Caelo	Octyldodecanol	14130206	12
Phönix	Octyldodecanol	14130206	1
Phoenix	Octyldodecanol	14130207	1
Caesar & Loretz	Octyldodecanol	14130207	1
Caelo	Octyldodecanol	14158402	9
Caelo	Octyldodecanol	14135206	1
Caelo	Octyldodecanol	1431707	1
Caelo	Octyldodecanol	14158411	1
Phoenix	Octyldodecanol	14158411	1
Caelo	Octyldodecanol	14371703	1
Caelo	Octyldodecanol	14371705	3
Caelo	Octyldodecanol	143710706	1
sanacorp	Octyldodecanol	14371706	1
Caelo	Octyldodecanol	14371707	3
Caelo	Octyldodecanol	14371710	2
Noweda 10.07.2015	Octyldodecanol	14371714	1
Anzag/Henry Lamotte	Octyldodecanol	14371711	1
Caelo	Octyldodecanol	14371714	3
Caelo	Octyldodecanol	14371716	5
Sanacorp	Octyldodecanol	14371716	1
Fagron	Octyldodecanol	14E06-B02	4
Fagron	Octyldodecanol	14E06-B02-301705	2
Fagron	Octyldodecanol	14E06-B02-293745	1
Fagron	Octyldodecanol	14E06-B02-301706	1
Fagron	Octyldodecanol	14E06-B02-30170	1
Fagron	Octyldodecanol	14E06-B02-293746	1
Caelo	Octyldodecanol	15135205	1
Caelo	Octyldodecanol	15135206	24
caesar&lorenz,Phönix	Octyldodecanol	15135206	1
Caesar & Loretz GmbH	Octyldodecanol	15135206	1
Caelo	Octyldodecanol	15135207	4
Caelo	Octyldodecanol	15135213	21
Caelo	Octyldodecanol	15135212	3

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Supplier	Substance	Batch	Spectra
Noweda	Octyldodecanol	15135213	1
Caelo	Octyldodecanol	1538005	1
Caelo	Octyldodecanol	1538004	1
Phönix	Octyldodecanol	1538009	1
Caelo	Octyldodecanol	15383002	1
Caelo	Octyldodecanol	15383003	4
Caesar&Loretz GmbH	Octyldodecanol	15383004	1
Fagron	Octyldodecanol	15383004	1
Caelo	Octyldodecanol	15383005	16
Hustadt-Apotheke	Octyldodecanol	15383005	1
Caolo	Octyldodecanol	15383005	1
Caelo	Octyldodecanol	15383008	13
Caelo	Octyldodecanol	15383009	9
Phoenix	Octyldodecanol	15383009	1
Noweda	Octyldodecanol	15383009	1
Fagron	Octyldodecanol	15E06-B02-30170	1
Caelo	Octyldodecanol	16095502	1
Caelo	Octyldodecanol	16095503	6
Caesar & Loretz/AHC	Octyldodecanol	16095503	1
Phoenix	Octyldodecanol	16095503	1
Caesar & Loretz/Noweda	Octyldodecanol	16095503	1
Caelo	Octyldodecanol	16095507	5
Caelo	Octyldodecanol	16095506	1
GEHE	Octyldodecanol	16095507	1
Caelo	Octyldodecanol	17082015C	1
Caelo	Octyldodecanol	31101416	1
Caelo	Octyldodecanol	4214U-02875	1
Gehe	Octyldodecanol	1136017	1
Spangropharm	Octyldodecanol	11060317	1
Phönix 08.11.12	Octyldodecanol	11369021	1
Fargon	Octyldodecanol	11C14-N14	1
Fagron	Octyldodecanol	11J13-N05	5
Caelo	Octyldodecanol	12111303	1
Sanacorp	Octyldodecanol	12142726	1
Caelo	Octyldodecanol	12011401	1
Caelo	Octyldodecanol	12044009	1
Noweda	Octyldodecanol	1216551	1
Kehr	Octyldodecanol	12165519	1
Anzag	Octyldodecanol	12165519	1
AHD 09.04.2013	Octyldodecanol	12165521	1
Caelo	Octyldodecanol	1265515	1
Fagron	Octyldodecanol	12C21-N03	3
Fagron	Octyldodecanol	12J04-N01	3
Fagron	Octyldodecanol	12C31-N03	1
Phoenix/Fargon	Octyldodecanol	12J04-N01	1
Phönix Gotha	Octyldodecanol	13044002	1
Noweda	Octyldodecanol	13044005	1
Caelo	Octyldodecanol	13044005	13
Caelo	Octyldodecanol	13044004	1
Sanacorp	Octyldodecanol	13044005	2
Caelo	Octyldodecanol	13044007	7
Caelo	Octyldodecanol	13044009	12
Gehe 27.06.2013	Octyldodecanol	13044009	1
Caesar & Loretz/ Noweda	Octyldodecanol	13044009	1
Caesar/Noweda	Octyldodecanol	13044009	1
Noweda	Octyldodecanol	13044013	2
Gehe	Octyldodecanol	13044013	1
Noweda	Octyldodecanol	13044016	1
AHD, 09.10.2013	Octyldodecanol	13044016	1
Caesar&lorenz,Phoenix	Octyldodecanol	13044016	1

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Supplier	Substance	Batch	Spectra
Sanacorp	Octyldodecanol	13222002	1
Noweda	Octyldodecanol	13222003	1
Sanacorp	Octyldodecanol	13222003	4
Sanacorp	Octyldodecanol	13222008	1
Caelo	Octyldodecanol	13222005	4
Noweda	Octyldodecanol	13222008	1
Caesar & Loretz GmbH	Octyldodecanol	13222008	1
Cealo / Noweda	Octyldodecanol	13222008	1
Noweda	Octyldodecanol	13360002	1
Caesar&lorenz,Phoenix	Octyldodecanol	13360006	1
Sanacorp	Octyldodecanol	13360006	1
Krieger	Octyldodecanol	13360006	1
Fagron	Octyldodecanol	13E07-N03	3
Sanacorp	Octyldodecanol	13E07-N07	1
Caesar&lorenz,Phoenix	Octyldodecanol	14371711	1
Caelo	Octyldodecanol	2513A-02875	2
Caelo	Octyldodecanol	2xa13360002	1
Fagron	Octyldodecanol	CE11350022	2
Caelo	Octyldodecanol	4113A2875	1
Sanacorp	Octyldodecanol	AKD31	1
Caelo	Octyldodecanol	CE11350022	2
Caelo	Octyldodecanol	1098722	1
Caelo	Octyldodecanol	11060317	1
Sanacorp	Octyldodecanol	12165514	1
Sanacorp	Octyldodecanol	13044002	1
A.H.D.	Octyldodecanol	13044007	1
Caelo	Octyldodecanol	13044040	1
Gehe	Octyldodecanol	13360012	1
Gehe	Octyldodecanol	13360003	1
Noweda	Octyldodecanol	21022171/7	1

- 57 703 spectra from 332 *Apo-Ident* customers from a total of 19 963 batches from a further 328 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 *Octyldodecanol* 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 *Octyldodecanol* 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	34 184
Type B	0	96	0	63 498
Type C	0	728	10	57 703

The substance/substance group *Octyldodecanol* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 93.7500 %)
Type C	100.0000 % (> 99.5963 %)	98.6450 % (> 98.2385 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30867	31330	3.83	51.84
31330	31330	0.00	50.52
31753	31330	12.37	53.27
32958	31330	7.69	48.81

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Oleic acid**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 32471-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Oleic acid; Acidum oleicum; Acidum oleinicum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Oleic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Oleic acid	15298701	32471	40	1702061
Caelo	Oleic acid	163091	33076	40	20161212*

Validation samples

A total of 156 379 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 *Oleic acid*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Oleic acid*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Oleic acid	15298701	32475	40
Caelo	Oleic acid	15298701	32747	40

- 63 514 spectra from a total of 1476 batches from further 439 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 *Oleic acid*.
- 58 441 spectra from 332 *Apo-Ident* customers from a total of 20 092 batches from a further 329 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 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.

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 *Oleic 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 *Oleic 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	80	0	34 264
Type B	0	80	0	63 514
Type C	0	0	0	58 441

The substance/substance group *Oleic 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
32471	32471	0.00	58.64
33076	33076	0.00	55.74

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Oregano oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30669-2017-07-04
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:

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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
Caelo	Oregano oil	11247605	30669	40	20110829
Caelo	Oregano oil	13354002	31196	40	1502253
Caelo	Oregano oil	13354007	31302	40	20131028
Caelo	Oregano oil	13354006	31406	40	20131028
Caelo	Oregano oil	14242905	31788	40	20140904

Validation samples

A total of 156 379 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 *Oregano oil*. These samples are listed above in the [calibration samples](#) section.
- 34 144 spectra from a total of 793 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Oregano oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Oregano oil	14242905	31788 [†]	20
Caelo	Oregano oil	16011001	32070	60

- 63 514 spectra from a total of 1475 batches from further 439 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 *Oregano oil*.

Supplier	Substance	Batch	Spectra
Noweda/Taoasis	Oregano oil	43878A-123313	1
Caelo	Oregano oil	12347604	1

[†]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*.

- 58 439 spectra from 332 *Apo-Ident* customers from a total of 20 090 batches from a further 328 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	200	0	34 144
Type B	0	80	0	63 514
Type C	0	2	0	58 439

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 % (> 99.9690 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.6008 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30669	31196	6.53	63.22
31196	31196	0.00	59.13
31302	31196	2.93	59.35
31406	31196	6.46	62.92
31788	31196	8.18	59.76

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Paraffin classification
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30874-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Paraffin classification; Emulsifying hydrophobic base gel DAC; Eye ointment, emulsifying DAC; Eye paraffin; Fatty ointment anhydrous, washable; Gelatum basalis hydrophobicum; Gelatum basalis hydrophobicum emulsificans; Hydrophilic ointment DAB; Hydrophobic base gel DAC; Lanae alcoholum unguentum; Oculentum emulsificans; Paraffin; Paraffin, white; Paraffin, yellow; Paraffinum; Unguentum alcoholum lanae; Unguentum alcoholum lanae SR; Unguentum Cordes®; Unguentum emulsificans DAB; Unguentum ophthalmicum emulsificans; Vaseline album; Vaseline album pro ophthalmicum; Vaseline flavum; Wool alcohol ointment DAB; Wool alcohol ointment SR with white paraffin; Wool alcohol ointment SR/DAC

Special notes

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

- Advice for the identification of water: Paraffin, liquid and paraffin, light liquid can not be conclusively distinguished by spectral analysis. An additional analysis of identity may be required.

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Paraffin classification*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Paraffin	12102101	30874	40	20120416
Caelo	Paraffin	12324307	30877	40	20121031
Caelo	Hydrophobic base...	12229003	30932	40	1405121
Caelo	Emulsifying hydr...	12343501	30933	40	1405098
Caelo	Paraffin, white	12374502	31009	40	20130102
Caelo	Paraffin, white	12032413	31010	40	20120203
Caelo	Hydrophobic base...	13299604	31168	40	20130909
apomix	Eye ointment, em...	15B241013	31174	39	1405331
Caelo	Wool alcohol oin...	12244302	31228	70	AR-15-FG-001376-01
Caelo	Wool alcohol oin...	14032501	31272	40	1507263
Hansen & Rose...	Hydrophobic base...	1023472	31292	40	20140328
Caelo	Paraffin	13248007	31351	40	AR-15-FG-002534-01
Caelo	Paraffin	13390602	31358	40	AR-15-FG-002530-01
Caelo	Paraffin, white	13341601	31437	40	20131108
Caelo	Wool alcohol oin...	14067001	31441	40	20140307
Caelo	Eye paraffin	13338710	31445	40	20131108
Caelo	Hydrophobic base...	14044601	31446	40	AR-15-FG-007940-01
Caelo	Hydrophilic oint...	14024802	31456	40	AR-14-FG-012697-01
Caelo	Paraffin, white	13268421	31468	40	20130823
Caelo	Paraffin, yellow	12321908	31473	40	AR-15-FG-002511-01
Euro OTC	Wool alcohol oin...	1211017-01	31522	40	AR-14-FG-012695-01
Euro OTC	Paraffin, yellow	1401017-01	31541	40	20140210
Caelo	Hydrophilic oint...	14024802	31567	40	20140129
Caelo	Emulsifying hydr...	14276401	31570	40	AR-15-FG-014916-01
Euro OTC	Paraffin, yellow	1401017-01	31586	40	20140210
Euro OTC	Paraffin	1409007-01	31587	40	20140929
Euro OTC	Paraffin, white	1405014-01	31590	40	20140702
Bombastus	Paraffin, white	290271	31601	40	20140929
Ichthyol	Fatty ointment a...	13A067	31602	40	1507406
Caelo	Eye paraffin	13338711	31610	40	AR-15-FG-008217-01
Caelo	Hydrophilic oint...	13245302	31611	40	20131008
Fagron	Hydrophilic oint...	14G08-T08-013954	31612	40	20140829
Euro OTC	Paraffin	1506021	31702	40	0000010380
Euro OTC	Paraffin, white	1509019	31736	60	20150929*
Euro OTC	Paraffin	1509011	31740	40	20150918*
apomix	Wool alcohol oin...	02A070515	31744	40	AR-16-FG-004495-01
Ichthyol	Fatty ointment a...	15A137	31807	40	20150804
Euro OTC	Paraffin	1511030	31812	40	20151208*
Euro OTC	Paraffin	1511029	31816	40	20151208*
Caelo	Hydrophilic oint...	154164	31909	40	20151215*
Caelo	Hydrophilic oint...	154165	31910	40	20151215*
Caelo	Paraffin, white	153276	31916	40	20151001*
Caelo	Paraffin, white	153368	31917	40	20151012*
Caelo	Emulsifying hydr...	153311	31920	40	20151006*
Caelo	Wool alcohol oin...	153347	31921	40	20150930*
Caelo	Paraffin, yellow	153304	31940	40	20151001*
Caelo	Paraffin, yellow	153305	31941	40	20151001*
apomix	Wool alcohol oin...	01A180215	31949	40	20150223
Ichthyol	Fatty ointment a...	15A150	31954	40	20150930
Caelo	Wool alcohol oin...	153421	31999	40	20151012*
Caelo	Wool alcohol oin...	153562	32017	40	20151028*
Euro OTC	Paraffin	1604009	32279	40	20160511*
Caelo	Paraffin, white	162274	32495	40	20160804*
Caelo	Wool alcohol oin...	162513	32517	40	20160907*
Euro OTC	Paraffin	1607039	32704	40	20160826*
Caelo	Eye paraffin	162718	32900	40	20161020*
apomix	Eye ointment, em...	06A090516	32946	40	20160517
apomix	Eye ointment, em...	10A041016	32947	40	20161017

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 2369 spectra of 58 reference samples from the substance/substance group *Paraffin classification*. These samples are listed above in the [calibration samples](#) section.
- 31 975 spectra from a total of 742 batches from further 213 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 3527 spectra of 98 reference samples from the substance/substance group *Paraffin classification*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Paraffin, white	90292119	30006	39
Caelo	Paraffin, white	10094704	30164	40
Ichthyol	Fatty ointment anhydrous, wa...	7A050	30218	50
Euro OTC	Wool alcohol ointment DAB	1007002-01	30269	40
Caelo	Emulsifying hydrophobic base...	10307401	30318	40
Ichthyol	Fatty ointment anhydrous, wa...	11A150	30375	30
Caelo	Hydrophilic ointment DAB	11211502	30393	40
Ichthyol	Fatty ointment anhydrous, wa...	11A070	30403	40
Ichthyol	Fatty ointment anhydrous, wa...	11A161	30424	40
Caelo	Eye paraffin	9274706	30434	40
Caelo	Paraffin, white	11374906	30466	70
Ichthyol	Fatty ointment anhydrous, wa...	11A139	30477	40
apomix	Eye ointment, emulsifying DAC	3B270212	30493	40
Caelo	Wool alcohol ointment SR wit...	11278101	30497	40
Ichthyol	Fatty ointment anhydrous, wa...	11A199	30587	20
Caelo	Hydrophilic ointment DAB	11211601	30609	40
Ichthyol	Fatty ointment anhydrous, wa...	11A202	30626	40
Caelo	Paraffin	13248007	31351 [†]	20
Caelo	Paraffin	13390602	31358 [†]	20
Caelo	Wool alcohol ointment SR wit...	14032501	31448	40
Euro OTC	Wool alcohol ointment DAB	1211017-01	31522 [†]	20
Euro OTC	Paraffin, yellow	1401017-01	31541 [†]	20
Caelo	Hydrophilic ointment DAB	14024802	31567 [†]	20
Caelo	Emulsifying hydrophobic base...	14276401	31570 [†]	20
Euro OTC	Paraffin, yellow	1401017-01	31586 [†]	20
Euro OTC	Paraffin	1409007-01	31587 [†]	20

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

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Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Paraffin, white	1405014-01	31590 [†]	20
Bombastus	Paraffin, white	290271	31601 [†]	20
Ichthyol	Fatty ointment anhydrous, wa...	13A067	31602 [†]	20
Caelo	Eye paraffin	13338711	31610 [†]	20
Caelo	Hydrophilic ointment DAB	13245302	31611 [†]	20
Fagron	Hydrophilic ointment DAB	14G08-T08-013954	31612 [†]	20
Euro OTC	Paraffin	1506021	31702 [†]	20
Euro OTC	Paraffin, white	1509019	31736 [†]	10
Euro OTC	Paraffin	1509011	31740 [†]	20
apomix	Wool alcohol ointment SR/DAC	2A070515	31744 [†]	20
Ichthyol	Fatty ointment anhydrous, wa...	15A137	31807 [†]	20
Euro OTC	Paraffin	1511030	31812 [†]	20
Euro OTC	Paraffin	1511029	31816 [†]	20
Caelo	Hydrophilic ointment DAB	154164	31909 [†]	20
Caelo	Hydrophilic ointment DAB	154165	31910 [†]	20
Caelo	Paraffin, white	153276	31916 [†]	20
Caelo	Paraffin, white	153368	31917 [†]	20
Caelo	Paraffin, white	153368	31918	60
Caelo	Paraffin, white	153497	31919	60
Caelo	Emulsifying hydrophobic base...	153311	31920 [†]	20
Caelo	Wool alcohol ointment SR wit...	153347	31921 [†]	20
Caelo	Paraffin, yellow	153304	31940 [†]	20
Caelo	Paraffin, yellow	153305	31941 [†]	20
Caelo	Paraffin, yellow	153306	31942	60
apomix	Wool alcohol ointment SR/DAC	1A180215	31949 [†]	20
Ichthyol	Fatty ointment anhydrous, wa...	15A150	31954 [†]	20
Caelo	Wool alcohol ointment DAB	153423	32011	60
Caelo	Wool alcohol ointment DAB	153424	32012	60
Caelo	Wool alcohol ointment DAB	153427	32013	60
Caelo	Wool alcohol ointment DAB	153428	32014	60
Caelo	Wool alcohol ointment DAB	153429	32015	60
Caelo	Wool alcohol ointment DAB	153558	32016	60
Caelo	Wool alcohol ointment DAB	153562	32017 [†]	20
Caelo	Wool alcohol ointment DAB	153563	32018	60
Caelo	Wool alcohol ointment DAB	153619	32019	60
Caelo	Wool alcohol ointment DAB	153618	32020	60
Caelo	Wool alcohol ointment DAB	153620	32021	48
Caelo	Wool alcohol ointment DAB	161102	32098	40
Caelo	Wool alcohol ointment DAB	161101	32099	40
Caelo	Wool alcohol ointment DAB	161103	32100	40
Caelo	Wool alcohol ointment DAB	161104	32101	40
Caelo	Wool alcohol ointment DAB	161105	32102	40
Caelo	Wool alcohol ointment DAB	161106	32103	40
Caelo	Wool alcohol ointment DAB	161107	32104	40
Euro OTC	Paraffin	1602026	32189	40
Euro OTC	Paraffin, white	1602009	32191	40
Caelo	Paraffin, white	161380	32223	40
Caelo	Paraffin, white	161380	32224	40
Euro OTC	Paraffin, white	1605019	32282	40
Euro OTC	Paraffin	1604045	32285	40
Caelo	Paraffin	161710	32323	40
Caelo	Hydrophilic ointment DAB	161668	32389	40
Caelo	Hydrophilic ointment DAB	161668	32390	40
Caelo	Hydrophilic ointment DAB	161670	32391	40
Euro OTC	Paraffin	1606032	32462	40
Caelo	Wool alcohol ointment DAB	162488	32511	40
Caelo	Wool alcohol ointment DAB	162488	32512	40
Caelo	Emulsifying hydrophobic base...	162259	32518	40
Caelo	Emulsifying hydrophobic base...	162260	32519	40

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Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Paraffin	1608007	32706	40
Euro OTC	Paraffin, white	1608041	32711	40
Euro OTC	Wool alcohol ointment DAB	1608040	32777	40
Euro OTC	Paraffin	1610017	32830	40
Caelo	Wool alcohol ointment DAB	162951	32864	40
Caelo	Wool alcohol ointment DAB	162952	32865	40
Caelo	Hydrophilic ointment DAB	162824	32866	40
Caelo	Hydrophilic ointment DAB	162825	32867	40
Caelo	Hydrophilic ointment DAB	162826	32868	40
Caelo	Hydrophilic ointment DAB	162827	32869	40
Caelo	Hydrophilic ointment DAB	162828	32870	40
Euro OTC	Paraffin, yellow	1701027	32987	40
Caelo	Hydrophobic base gel DAC	16151105	33223	40

- 60 067 spectra from a total of 1384 batches from further 428 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.

- 5961 spectra from 304 *Apo-Ident* customers from 1904 batches from the substance/substance group *Paraffin classification*.

Supplier	Substance	Batch	Spectra
PKH GmbH Halle	Eye ointment, emulsifying DAC	1C080114	1
Apomix / Sanacorp	Eye ointment, emulsifying DAC	6D090516	1
Apomix	Eye ointment, emulsifying DAC	2C040116	1
Apomix / Sanacorp	Eye ointment, emulsifying DAC	16A231014	1
Apomix	Eye ointment, emulsifying DAC	14A011013	1
apomix/Noweda	Eye ointment, emulsifying DAC	20D011215	1
AMH	Eye ointment, emulsifying DAC	16B011015	1
Noweda/apomix	Eye ointment, emulsifying DAC	1B070113	1
Apomix / Noweda	Eye ointment, emulsifying DAC	15A030815	1
Apomix/Noweda	Eye ointment, emulsifying DAC	17A231014	1
Caelo	Eye ointment, emulsifying DAC	3A180213	1
PHOENIX 03.03.2014	Eye ointment, emulsifying DAC	16B111113	1
Apomix / Phönix	Eye ointment, emulsifying DAC	7A210513	1
apomix/Phönix	Eye ointment, emulsifying DAC	9B25061	1
Alliance Healthcare/Apo...	Eye ointment, emulsifying DAC	17A111113	1
Caelo	Eye ointment, emulsifying DAC	13084905	1
PKH Halle / Noweda	Eye ointment, emulsifying DAC	7D210513	1
Apomix	Eye ointment, emulsifying DAC	11B030912	1
Phoenix	Eye paraffin	13338713	2
Caelo	Eye paraffin	13338713	8
Caelo	Eye paraffin	5011507	1
Caelo	Eye paraffin	6021505	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
Caelo	Eye paraffin	13338707	1
Gehe	Eye paraffin	13338704	1
Caelo	Eye paraffin	14124703	4
Caelo	Eye paraffin	14124704	3
Phoenix Goettin	Eye paraffin	14124704	1
Sanacorp	Eye paraffin	14124704	1
Caelo	Eye paraffin	14124705	5
Gehe	Eye paraffin	14124706	1
Caelo	Eye paraffin	14124706	4
Caelo	Eye paraffin	14124707	11
Caelo	Eye paraffin	14124708	2
Caelo	Eye paraffin	1412703	1
Caelo	Eye paraffin	14301804	6
Caesar & Loretz GmbH / ...	Eye paraffin	14301804	1
Caelo	Eye paraffin	14301805	5
Caelo	Eye paraffin	14301806	1
Caesar & Loretz/Noweda	Eye paraffin	150500004	1
Caelo	Eye paraffin	15050002	15
Caelo	Eye paraffin	15050003	4
Caelo	Eye paraffin	15050004	3
Caelo	Eye paraffin	15050005	6
Caelo	Eye paraffin	15050007	1
Caelo	Eye paraffin	15278801	7
Caelo	Eye paraffin	1505003	1
Caelo	Eye paraffin	15278803	1
Caelo	Eye paraffin	15278804	4
Caelo	Eye paraffin	1527880	1
Caelo	Eye paraffin	15278805	6
Caelo	Eye paraffin	15278809	2
Ebert & Jacobi 31.05...	Eye paraffin	15278809	1
Caelo	Eye paraffin	15278808	2
Caelo	Eye paraffin	15441501	6
Caelo	Eye paraffin	15441502	5
Caelo	Eye paraffin	15441505	6
Ebert u. Jacobi 20.07...	Eye paraffin	15441505	1
Caelo	Eye paraffin	15441506	1
Caelo	Eye paraffin	15441509	4
Caelo	Eye paraffin	15441510	1
Caelo	Eye paraffin	15441511	1
Caelo	Eye paraffin	19/AKD2	1
Caelo	Eye paraffin	20101401	1
Caelo	Eye paraffin	24031503	1
Caelo	Eye paraffin	19051504	1
Sanacorp	Eye paraffin	19/AKD4	1
Caelo	Eye paraffin	31071502	1
Caelo	Eye paraffin		1
Caelo	Eye paraffin	29101401	1
Fagron	Eye paraffin	790619-021159	3
Fagron	Eye paraffin	790619-013771	1
Caelo	Paraffin, white		3
gehe	Hydrophobic base gel DAC	10L14-T54-006109	3
Caelo	Hydrophobic base gel DAC	14044601	7
Caelo	Hydrophobic base gel DAC	14087501	1
Caelo	Hydrophobic base gel DAC	14102502	2
Caelo	Hydrophobic base gel DAC	13341703	3
Caelo	Hydrophobic base gel DAC	14158002	4
Caelo	Hydrophobic base gel DAC	14158003	7
Caelo	Hydrophobic base gel DAC	14276401	3
Caelo	Hydrophobic base gel DAC	15055705	3
Caelo	Hydrophobic base gel DAC	14158006	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrophobic base gel DAC	15064101	7
Caelo	Hydrophobic base gel DAC	15240805	5
Caelo	Hydrophobic base gel DAC	15064201	1
Caelo	Hydrophobic base gel DAC	15149603	3
Caelo	Hydrophobic base gel DAC	15436103	1
Caelo	Hydrophobic base gel DAC	15269201	1
Caelo	Hydrophobic base gel DAC	16070503	7
Caesar & Loretz GmbH Hi...	Hydrophobic base gel DAC	16070503	2
Caelo	Hydrophobic base gel DAC	282094	1
Caelo	Hydrophobic base gel DAC	286013	2
Bombastus	Hydrophobic base gel DAC	28111403	1
Phoenix	Hydrophobic base gel DAC	10L14-T54	2
Bombastus	Hydrophobic base gel DAC	282094	3
Bombastus	Hydrophobic base gel DAC	294418	1
Caelo	Hydrophobic base gel DAC	12229001	2
Fagron	Hydrophobic base gel DAC	11K23-T01	1
Bombastus	Hydrophobic base gel DAC	289214	4
Fagron	Hydrophobic base gel DAC	10L14-T54-000713	1
Caelo	Hydrophobic base gel DAC	12229005	1
Caelo	Hydrophobic base gel DAC	12362503	3
11.07.13	Hydrophobic base gel DAC	12324704	1
Caelo	Hydrophobic base gel DAC	12362504	2
Caelo	Hydrophobic base gel DAC	123662505	1
Caelo	Hydrophobic base gel DAC	12362505	3
Euro OTC	Hydrophobic base gel DAC	12362505	1
Caelo	Hydrophobic base gel DAC	13085004	3
Caelo	Hydrophobic base gel DAC	13165201	1
Caesar & Loretz GmbH, 4...	Hydrophobic base gel DAC	13165201	1
Caelo	Hydrophobic base gel DAC	13299604	9
Caelo	Hydrophobic base gel DAC	13295801	1
Sanacorp	Hydrophobic base gel DAC	AKD18	1
Bombastus	Hydrophobic base gel DAC	279074	3
Bombastus	Hydrophobic base gel DAC	277443	1
Caelo	Emulsifying hydrophobic base...	30071201	1
15.07.13	Hydrophobic base gel DAC	277443	3
Sanacorp	Fatty ointment anhydrous, wa...	103/AKD1	1
Ichthyol	Fatty ointment anhydrous, wa...	7011501	1
Ichthyol	Fatty ointment anhydrous, wa...	4091516	1
Caelo	Fatty ointment anhydrous, wa...	13A042	2
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	12A118	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	13A068	2
ichthyol-gesellschaft	Fatty ointment anhydrous, wa...	13A068	2
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	13A067	1
Ichthyol	Fatty ointment anhydrous, wa...	13041504	1
Caelo	Fatty ointment anhydrous, wa...	13A090	2
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A090	2
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	13A089	1
Alliance Health 11.03.14	Fatty ointment anhydrous, wa...	13A090	1
Caesar & Loretz GmbH Hi...	Fatty ointment anhydrous, wa...	13A090	1
Ichthyol / Phoenix	Fatty ointment anhydrous, wa...	13A090	1
ichthyol/Sanacorp	Fatty ointment anhydrous, wa...	13A090	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A089	1
ichthyol/Gehe	Fatty ointment anhydrous, wa...	13A091	1
Noweda	Fatty ointment anhydrous, wa...	13A091	1
IchthyolSanacorp	Fatty ointment anhydrous, wa...	13A110	1
Ichthyol	Fatty ointment anhydrous, wa...	13A138	2
Caelo	Fatty ointment anhydrous, wa...	13A136	1
Ichthyol	Fatty ointment anhydrous, wa...	13A140	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	13A140	1
Phoenix/Ichthyol	Fatty ointment anhydrous, wa...	13A140	1

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Supplier	Substance	Batch	Spectra
Ichthyol	Fatty ointment anhydrous, wa...	13A142	1
Ichthyol	Fatty ointment anhydrous, wa...	13A141	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	13A142	3
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	13A142	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	13A153	1
Ichthyol	Fatty ointment anhydrous, wa...	13A153	1
Gehe	Fatty ointment anhydrous, wa...	13A156	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A156	1
Caelo	Fatty ointment anhydrous, wa...	13A157	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	13A156	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	13A156	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A158	1
Berkel AHK	Fatty ointment anhydrous, wa...	13A158	1
Ichthyol/Ebert	Fatty ointment anhydrous, wa...	13A159	1
Ichthyol	Fatty ointment anhydrous, wa...	13A159	2
Gehe	Fatty ointment anhydrous, wa...	13A159	1
Sanacorp	Fatty ointment anhydrous, wa...	13A159	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	13A166	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	13A166	3
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	13A166	1
Ichthyol/Otto	Fatty ointment anhydrous, wa...	13A159	1
Ichthyol über Phoenix	Fatty ointment anhydrous, wa...	13A166	1
Ichthyol	Fatty ointment anhydrous, wa...	13A166	1
Caelo	Fatty ointment anhydrous, wa...	13A172	1
Ichthyol	Fatty ointment anhydrous, wa...	13A171	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	13A170	1
Ichthyol	Fatty ointment anhydrous, wa...	13A172	1
Caelo	Fatty ointment anhydrous, wa...	13A171	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A172	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	13A178	1
Ichthyol	Fatty ointment anhydrous, wa...	13A178	2
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	13A172	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	13A178	3
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	13A180	2
Ichthyol	Fatty ointment anhydrous, wa...	13A180	1
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	13A181	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	13A181	1
Anzag/Ichthyol	Fatty ointment anhydrous, wa...	13A180	1
Ichthyol Gesellschaft/ ...	Fatty ointment anhydrous, wa...	13A181	1
Ichthyol -Gesellschaft	Fatty ointment anhydrous, wa...	13A181	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	13A181	2
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	13A216	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A181	1
Gehe/Ichthyol	Fatty ointment anhydrous, wa...	13A090	1
Ichthyol	Fatty ointment anhydrous, wa...	14031409	1
ANZAG/Ichthyol Gesellsc...	Fatty ointment anhydrous, wa...	13A72	1
Ichthyol-Gesellschaft/ ...	Fatty ointment anhydrous, wa...	14A005	1
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	1415A-02532	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	14A006	1
Ichthyol Cordes/Allianc...	Fatty ointment anhydrous, wa...	14A009	1
Caelo	Fatty ointment anhydrous, wa...	14A009	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	14A009	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	14A055	4
Cordes	Fatty ointment anhydrous, wa...	14A055	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	14A056	2
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	14A047	1
Gehe	Fatty ointment anhydrous, wa...	14A056	1
Berkel AHK	Fatty ointment anhydrous, wa...	14A056	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	14A057	1
Stumpf/Ichthyol	Fatty ointment anhydrous, wa...	14A057	1

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Supplier	Substance	Batch	Spectra
Ichthyol	Fatty ointment anhydrous, wa...	14A057	3
Bombastus	Fatty ointment anhydrous, wa...	14A060	1
sanacorp	Fatty ointment anhydrous, wa...	14A060	1
Ichthyol	Fatty ointment anhydrous, wa...	14A061	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	14A061	1
Gehe/Ichthyol	Fatty ointment anhydrous, wa...	14A061	1
Gehe/Ichthyol	Fatty ointment anhydrous, wa...	14A062	3
Cordes	Fatty ointment anhydrous, wa...	14A062	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	14A062	1
Ichthyol über Phoenix	Fatty ointment anhydrous, wa...	14A062	1
Caelo	Fatty ointment anhydrous, wa...	14A063	2
Stumpf/Ichtyol	Fatty ointment anhydrous, wa...	14A063	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	14A063	1
Ichthyol	Fatty ointment anhydrous, wa...	14A063	1
Euro OTC	Fatty ointment anhydrous, wa...	14A078	2
Euro OTC	Fatty ointment anhydrous, wa...	14A079	2
Caelo	Fatty ointment anhydrous, wa...	14A079	1
Ichthyol / E	Fatty ointment anhydrous, wa...	14A079	1
Ichtyol-Gesellschaft	Fatty ointment anhydrous, wa...	14A079	1
Caelo	Fatty ointment anhydrous, wa...	14A078	1
Alliance health	Fatty ointment anhydrous, wa...	14A079	1
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	14A079	1
Ichtyol-Gesellschaft/Ph...	Fatty ointment anhydrous, wa...	14A095	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	14A095	1
Ichthyol-Gesellschaft/P...	Fatty ointment anhydrous, wa...	14A095	2
Ichtyol/Sanacorp	Fatty ointment anhydrous, wa...	14A097	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	14A095	1
Ichthyol	Fatty ointment anhydrous, wa...	14A098	1
Ichthyol	Fatty ointment anhydrous, wa...	14A113	1
Caelo	Fatty ointment anhydrous, wa...	14A113	1
Ichthyol/Otto	Fatty ointment anhydrous, wa...	14A113	1
Ichthyol	Fatty ointment anhydrous, wa...	14A114	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	14A112	1
Cealo	Fatty ointment anhydrous, wa...	14A113	1
ICHTHYOL	Fatty ointment anhydrous, wa...	14A114	1
Ichthyol über Phoenix	Fatty ointment anhydrous, wa...	14A114	1
Ichthyol-Gesellschaft/P...	Fatty ointment anhydrous, wa...	14a114	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	14A115	1
phönix	Fatty ointment anhydrous, wa...	14A116	1
AHD	Fatty ointment anhydrous, wa...	14A117	1
Cordes	Fatty ointment anhydrous, wa...	14A117	2
Caelo	Fatty ointment anhydrous, wa...	14A116	1
Ichthyol / Sanacorp	Fatty ointment anhydrous, wa...	14A168	1
Ichthyol	Fatty ointment anhydrous, wa...	14A132	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	14A117	1
ICHTHYOL	Fatty ointment anhydrous, wa...	14A171	1
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	14A172	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	14A130	1
Ichthyol / Sanacorp	Fatty ointment anhydrous, wa...	14A172	1
Sanacorp	Fatty ointment anhydrous, wa...	14A172	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	14A172	1
Ichthyol- Gesellschaft ...	Fatty ointment anhydrous, wa...	14A172	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	14A172	2
ichthyol	Fatty ointment anhydrous, wa...	14A172	1
Ichthyol	Fatty ointment anhydrous, wa...	14A172	1
Ichthyol/ Noweda	Fatty ointment anhydrous, wa...	14A172	1
Ichthyol	Fatty ointment anhydrous, wa...	14A173	1
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	14A173	1
Caelo	Fatty ointment anhydrous, wa...	14A312	1
Ichthyol/Otto	Fatty ointment anhydrous, wa...	15A010	1

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Supplier	Substance	Batch	Spectra
ICHTHYOL/GEHE	Fatty ointment anhydrous, wa...	15A011	1
Fagron	Fatty ointment anhydrous, wa...	15A010	1
ICHTHYOL Gesellschaft /...	Fatty ointment anhydrous, wa...	15A020	1
Caelo	Fatty ointment anhydrous, wa...	14A213	1
Ichthyol-Gesellschaft /...	Fatty ointment anhydrous, wa...	15A020	2
Fagron	Fatty ointment anhydrous, wa...	15A020	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	15A020	1
Ichthyol / G	Fatty ointment anhydrous, wa...	15A020	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	15A020	1
Gehe Kassel	Fatty ointment anhydrous, wa...	15A021	1
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	15A021	1
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	15a021	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	15A022	1
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	15A022	1
Ichthyol	Fatty ointment anhydrous, wa...	15A022	1
Ichthyol-Gesellschaft /...	Fatty ointment anhydrous, wa...	15A023	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	15A027	2
Ichthyol, Noweda	Fatty ointment anhydrous, wa...	15A023	1
Caelo	Fatty ointment anhydrous, wa...	15A040	1
Gehe,11.05.15/Cordes	Fatty ointment anhydrous, wa...	15A040	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	15A040	2
Ichthyol	Fatty ointment anhydrous, wa...	15A040	2
Ichthyol über Phoenix	Fatty ointment anhydrous, wa...	15A042	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	15A042	1
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	15A042	1
SANOVA	Fatty ointment anhydrous, wa...	15A044	1
Caelo	Fatty ointment anhydrous, wa...	15A060	1
Ichthyol-Gesellschaft C...	Fatty ointment anhydrous, wa...	15A061	1
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	15A060	1
Caelo	Fatty ointment anhydrous, wa...	15A062	2
Noweda	Fatty ointment anhydrous, wa...	15A062	1
IchthyolSanacorp	Fatty ointment anhydrous, wa...	15A076	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	15A074	1
Ichthyol	Fatty ointment anhydrous, wa...	15A079	1
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	15A090	1
Ichthyol-Gesellschaft /...	Fatty ointment anhydrous, wa...	15A073	2
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	15A073	1
Caelo	Fatty ointment anhydrous, wa...	15A073	1
ICHTHYOL	Fatty ointment anhydrous, wa...	15a089	1
Ichthyol Gesellschaft/ ...	Fatty ointment anhydrous, wa...	15A087	1
Ichthyol	Fatty ointment anhydrous, wa...	15A091	2
Caelo	Fatty ointment anhydrous, wa...	15A089	1
ICHTHYOL-GESELLSCHAFT C...	Fatty ointment anhydrous, wa...	15A073	1
Ichthyol/Otto	Fatty ointment anhydrous, wa...	15A107	1
Caelo	Fatty ointment anhydrous, wa...	15A092	1
Caelo	Fatty ointment anhydrous, wa...	15A091	1
Noweda	Fatty ointment anhydrous, wa...	15A123	1
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	15A123	3
Ichthyol-Gesellschaft /...	Fatty ointment anhydrous, wa...	15A124	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	15A124	1
Fiebig/Ichthyol	Fatty ointment anhydrous, wa...	15A124	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	15A123	1
Caelo	Fatty ointment anhydrous, wa...	15A137	2
ichthyol	Fatty ointment anhydrous, wa...	15A139	1
Ichtyol/Phoenix	Fatty ointment anhydrous, wa...	15A137	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	15A142	1
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	15A148	1
VDL	Fatty ointment anhydrous, wa...	15A140	1
Ichthyol	Fatty ointment anhydrous, wa...	15A156	1
Ichthyol/Sanova Pharma	Fatty ointment anhydrous, wa...	15A156	1

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Supplier	Substance	Batch	Spectra
Ichthyol	Fatty ointment anhydrous, wa...	15A150	1
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	15A159	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	15A191	1
Noweda	Fatty ointment anhydrous, wa...	15A191	1
Caelo	Fatty ointment anhydrous, wa...	15A191	1
Ichthyol	Fatty ointment anhydrous, wa...	15A191	1
Phönix	Fatty ointment anhydrous, wa...	16A048	1
Caelo	Fatty ointment anhydrous, wa...	16/082/C	1
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	15A195	1
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	16A048	1
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	15A191	1
SANOVA	Fatty ointment anhydrous, wa...	16A045	1
Ichthyol	Fatty ointment anhydrous, wa...	16A045	1
Ichthyol	Fatty ointment anhydrous, wa...	16A048	1
Caelo	Fatty ointment anhydrous, wa...	16A051	1
Ichthyol über Phoenix	Fatty ointment anhydrous, wa...	16A058	1
Ichthyol	Fatty ointment anhydrous, wa...	16A058	1
Euro OTC	Fatty ointment anhydrous, wa...	16A074	1
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	16A085	1
Caelo	Fatty ointment anhydrous, wa...	16A099	1
Cordes/Noweda	Fatty ointment anhydrous, wa...	16A101	1
Bombastus	Fatty ointment anhydrous, wa...	16A099	1
Ichthyol über Phoenix	Fatty ointment anhydrous, wa...	16A119	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	16A099	1
Phoenix	Fatty ointment anhydrous, wa...	16A121	1
Caelo	Fatty ointment anhydrous, wa...	16A122	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	16A139	1
Ichthyol/Noweda 31.01.2017	Fatty ointment anhydrous, wa...	16A140	1
Caelo	Fatty ointment anhydrous, wa...	16A140	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	4913Q-02532	1
gebepharm	Fatty ointment anhydrous, wa...	913I-02532	1
Ichthyol	Fatty ointment anhydrous, wa...	414022-2-P	1
Caelo	Fatty ointment anhydrous, wa...	913M-02532	1
Phönix /Ichthyol	Fatty ointment anhydrous, wa...	Ch13A089	1
Ichthyol	Fatty ointment anhydrous, wa...	16A173	1
Caelo	Fatty ointment anhydrous, wa...	9A163	1
Ichthyol	Fatty ointment anhydrous, wa...	11a042	1
Ichthyol - Gesellschaft	Fatty ointment anhydrous, wa...	11A085	1
Ichthyol	Fatty ointment anhydrous, wa...	11A085	3
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	11A171	1
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	11A042	1
Ichthyol	Fatty ointment anhydrous, wa...	11A118	2
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	11A146	1
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	11A187	1
Kehr	Fatty ointment anhydrous, wa...	11A187	1
ICHTHYOL-GESELLSCHAFT C...	Fatty ointment anhydrous, wa...	11A187	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	11A177	1
Ichthyol-Gesellschaft C...	Fatty ointment anhydrous, wa...	11A199	1
CIchthyol/K	Fatty ointment anhydrous, wa...	11A199	1
Ichthyol-Gesellschaft / K	Fatty ointment anhydrous, wa...	11A202	1
Gehe	Fatty ointment anhydrous, wa...	11A223	2
Phönix Gotha	Fatty ointment anhydrous, wa...	11A234	1
IchthyolAnzag 10.05.2012	Fatty ointment anhydrous, wa...	11A234	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	11A202	1
Noweda	Fatty ointment anhydrous, wa...	11A227	1
ICHTHYOL-GESELLSCHAFT	Fatty ointment anhydrous, wa...	11A202	1
Ichthyol/Otto	Fatty ointment anhydrous, wa...	12A020	1
Caelo	Fatty ointment anhydrous, wa...		1
Ichthyol	Fatty ointment anhydrous, wa...	11A233	1
Phönix	Fatty ointment anhydrous, wa...	12A049	1

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Supplier	Substance	Batch	Spectra
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	12A054	1
Phoenix	Fatty ointment anhydrous, wa...	12A056	1
Ichtyol-Gesellschaft/Ph...	Fatty ointment anhydrous, wa...	12A058	1
Caelo	Fatty ointment anhydrous, wa...	12A022	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	12A058	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	12A060	2
Ichthyol / Anzag	Fatty ointment anhydrous, wa...	12A079	1
Ichthyol	Fatty ointment anhydrous, wa...	12A078	1
Cordes	Fatty ointment anhydrous, wa...	12A079	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	12A064	1
Ichthyol-Gesellschaft / G	Fatty ointment anhydrous, wa...	12A064	1
Anzag	Fatty ointment anhydrous, wa...	12A077	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	12A079	1
Ichthyol	Fatty ointment anhydrous, wa...	12A102	2
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	12A102	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	12A115	2
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	12A102	1
Ichthyol	Fatty ointment anhydrous, wa...	12A115	3
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	12A115	1
Ichthyol/Krieger	Fatty ointment anhydrous, wa...	12A102	1
Ichthyol-Gesellschaft C...	Fatty ointment anhydrous, wa...	12A115	1
Ichthyol-Gesellschaft / G	Fatty ointment anhydrous, wa...	12A118	2
Ichthyol / Phoenix Leip...	Fatty ointment anhydrous, wa...	12A118	1
Ichthyol-Gesellschaft / G	Fatty ointment anhydrous, wa...	12A123	1
Ichthyol	Fatty ointment anhydrous, wa...	12A121	2
Noweda/ Ichtyol	Fatty ointment anhydrous, wa...	12A124	1
Sanacorp	Fatty ointment anhydrous, wa...	12A129	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	12A123	1
Cordes	Fatty ointment anhydrous, wa...	12A123	1
Ichthyol/Otto	Fatty ointment anhydrous, wa...	12A130	2
Noweda	Fatty ointment anhydrous, wa...	12A123	1
Anzag	Fatty ointment anhydrous, wa...	12A130	1
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	12A130	1
Sanova	Fatty ointment anhydrous, wa...	12A130	1
Ichthyol/ Cordes	Fatty ointment anhydrous, wa...	12A139	1
Ichthyol	Fatty ointment anhydrous, wa...	12A131	2
Phönix	Fatty ointment anhydrous, wa...	12A131	1
Phönix/Ichthyol	Fatty ointment anhydrous, wa...	12A139	1
ichthyol	Fatty ointment anhydrous, wa...	12A139	1
Caelo	Fatty ointment anhydrous, wa...	12A146	1
Corde	Fatty ointment anhydrous, wa...	12a152	1
Ichthyol	Fatty ointment anhydrous, wa...	12a145	1
ichthyol	Fatty ointment anhydrous, wa...	12A152	1
IchthyolGesellschaft Co...	Fatty ointment anhydrous, wa...	12A152	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	12A152	2
Maros / Phoenix	Fatty ointment anhydrous, wa...	12A152	1
Ichthyol	Fatty ointment anhydrous, wa...	12A152	1
ICHTHYOL-GES/GEHE	Fatty ointment anhydrous, wa...	12A152	1
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	12A152	1
Fagron	Fatty ointment anhydrous, wa...	12A152	1
Caelo	Fatty ointment anhydrous, wa...	12A152	1
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	12A152	2
Ichthyol	Fatty ointment anhydrous, wa...	12a152	1
Gehe	Fatty ointment anhydrous, wa...	12A155	1
Ichthyol-Gesellschaft / E	Fatty ointment anhydrous, wa...	12A152	1
Cordes	Fatty ointment anhydrous, wa...	12A155	1
ICHTHYOL-GESELLSCHAFT	Fatty ointment anhydrous, wa...	12A155	1
Gehe	Fatty ointment anhydrous, wa...	12a155	2
phönix/Ichthyol-Gesells...	Fatty ointment anhydrous, wa...	12A156	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	12A156	1

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Supplier	Substance	Batch	Spectra
Caelo	Fatty ointment anhydrous, wa...	12A156	1
Ichthyol	Fatty ointment anhydrous, wa...	12A157	1
Sanacorp	Fatty ointment anhydrous, wa...	12A160	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	12A183	1
Ichthyol	Fatty ointment anhydrous, wa...	12A160	1
Ichthyol-Gesellschaft/V...	Fatty ointment anhydrous, wa...	12A183	1
Caelo	Fatty ointment anhydrous, wa...	12A183	2
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	12A183	1
IchthyolGesellschaft Co...	Fatty ointment anhydrous, wa...	12A183	1
Gehe	Fatty ointment anhydrous, wa...	12A183	1
Noweda	Fatty ointment anhydrous, wa...	12A183	2
Ichthyol / Sanacorp	Fatty ointment anhydrous, wa...	12A183	1
ichthyol/Sanacorp	Fatty ointment anhydrous, wa...	12A183	1
Ichthyol-Gesellschaft C...	Fatty ointment anhydrous, wa...	12A183	1
Ichthyol/ Noweda	Fatty ointment anhydrous, wa...	12A183	1
Ichthyol / Phoenix	Fatty ointment anhydrous, wa...	12A183	1
ICHTHYOL-Gesellschaft	Fatty ointment anhydrous, wa...	12A184	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	12A184	1
Ichthyol-Gesellschaft C...	Fatty ointment anhydrous, wa...	12A184	1
Sanacorp	Fatty ointment anhydrous, wa...	12a184	1
Ichthyol/Krieger	Fatty ointment anhydrous, wa...	12A184	1
Ichthyol-Ges	Fatty ointment anhydrous, wa...	12A184	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	12A184	1
ICHTHYOL-GESELLSCHAFT	Fatty ointment anhydrous, wa...	12A184	1
Ichthyol	Fatty ointment anhydrous, wa...	12A185	1
Ichthy	Fatty ointment anhydrous, wa...	12A185	1
Ichthyol/AHD	Fatty ointment anhydrous, wa...	12A185	1
ICHTHYOL-GESELLSCHAFT C...	Fatty ointment anhydrous, wa...	12A185	1
Caelo	Fatty ointment anhydrous, wa...	12A185	1
Phoenix 26.11.12	Fatty ointment anhydrous, wa...	12A185	1
ichthyol	Fatty ointment anhydrous, wa...	12A190	1
Stumpf/Ichthyol	Fatty ointment anhydrous, wa...	12A190	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	12A190	1
Ichthyol	Fatty ointment anhydrous, wa...	12A190	1
Gehe	Fatty ointment anhydrous, wa...	12A205	2
Ichthyol/ Cordes	Fatty ointment anhydrous, wa...	12A205	1
Ichthyol	Fatty ointment anhydrous, wa...	12A205	2
Ichthyol	Fatty ointment anhydrous, wa...	12A206	1
Caelo	Fatty ointment anhydrous, wa...	12A206	4
Ichthyol	Fatty ointment anhydrous, wa...	12a205	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	12A206	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	12A205	1
Phönix	Fatty ointment anhydrous, wa...	12A211	1
ichthyol	Fatty ointment anhydrous, wa...	12A206	1
Sanacorp / Ichthyol	Fatty ointment anhydrous, wa...	12A206	1
Ichthyol	Fatty ointment anhydrous, wa...	12A211	1
Ichthyol/Otto	Fatty ointment anhydrous, wa...	12AI30	1
Caelo	Fatty ointment anhydrous, wa...	131A043	1
Ichthyol	Fatty ointment anhydrous, wa...	13A005	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	13A006	1
Ichthyol	Fatty ointment anhydrous, wa...	13A003	1
Großhandel	Fatty ointment anhydrous, wa...	13A010	1
Ichthyol,Noweda	Fatty ointment anhydrous, wa...	13a009	2
Cordes	Fatty ointment anhydrous, wa...	13a025	1
Ichthyol	Fatty ointment anhydrous, wa...	13A015	1
Ichthyol	Fatty ointment anhydrous, wa...	13A010	2
Ichthyol	Fatty ointment anhydrous, wa...	13A006	1
IchthyolSanacorp	Fatty ointment anhydrous, wa...	13A025	1
Ichthyol	Fatty ointment anhydrous, wa...	13A029	2
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	13A029	1

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Supplier	Substance	Batch	Spectra
Anzag/ Ichthyol	Fatty ointment anhydrous, wa...	13A029	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	13A030	1
Ichthyol	Fatty ointment anhydrous, wa...	13A030	2
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	13A031	1
Ichthyol	Fatty ointment anhydrous, wa...	13A031	2
Gehe	Fatty ointment anhydrous, wa...	13A031	3
ICHTHYOL/11	Fatty ointment anhydrous, wa...	13A031	1
ichthyol	Fatty ointment anhydrous, wa...	13A032	1
Alliance Health	Fatty ointment anhydrous, wa...	13A032	1
Ichthyol	Fatty ointment anhydrous, wa...	13A032	2
Phönix Gotha	Fatty ointment anhydrous, wa...	13A032	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	13A033	1
Phönix	Fatty ointment anhydrous, wa...	13A034	1
Ichthyol	Fatty ointment anhydrous, wa...	13A034	2
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	13A034	1
Ichthyol-Gesellschaft, ...	Fatty ointment anhydrous, wa...	13A034	1
Ichthyol/phönix	Fatty ointment anhydrous, wa...	13A034	1
	Fatty ointment anhydrous, wa...	13A034	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A042	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	13A034	1
Ichthyol/ebert	Fatty ointment anhydrous, wa...	13A034	1
Gehe/Ichthyol	Fatty ointment anhydrous, wa...	13A042	1
Ichthyol	Fatty ointment anhydrous, wa...	13A042	1
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	13A042	1
Bombastus	Fatty ointment anhydrous, wa...	13A042	1
Ichthyol	Fatty ointment anhydrous, wa...	13A043	2
Ichthyol-Gesellschaft / G	Fatty ointment anhydrous, wa...	13A042	1
Caelo	Fatty ointment anhydrous, wa...	13A043	1
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	13A043	1
ICHTHYOL-GESELLSCHAFT	Fatty ointment anhydrous, wa...	13A043	1
Ichthyol/ Noweda	Fatty ointment anhydrous, wa...	13A043	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A042	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A043	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	13A042	1
Ichthyol	Fatty ointment anhydrous, wa...	13A047	2
Ichthyol	Fatty ointment anhydrous, wa...	13A043	1
Ichthyol/Alliance healt...	Fatty ointment anhydrous, wa...	13A047	1
ichthyol/ANZAG	Fatty ointment anhydrous, wa...	13A047	1
cordes/phoenix	Fatty ointment anhydrous, wa...	13A047	1
Gehe	Fatty ointment anhydrous, wa...	13A047	1
Ichthyol	Fatty ointment anhydrous, wa...	13A048	1
Caelo	Fatty ointment anhydrous, wa...	13A049	1
Jenne	Fatty ointment anhydrous, wa...	13A049	1
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	13A049	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	13A050	1
Ichthyol	Fatty ointment anhydrous, wa...	13A050	4
Ichthyol-Gesellschaft, ...	Fatty ointment anhydrous, wa...	13A050	1
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	13A049/13A050	1
Cordes/Phönix	Fatty ointment anhydrous, wa...	13A050	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	13A051	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	13A051	1
Stumpf/Ichthyol	Fatty ointment anhydrous, wa...	13A051	1
phönix	Fatty ointment anhydrous, wa...	13A051	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	13A051	1
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	13A051	1
Ebert/Ichthyol	Fatty ointment anhydrous, wa...	13A052	1
ichthyol gesellschaft	Fatty ointment anhydrous, wa...	13A051	1
Ichthyol	Fatty ointment anhydrous, wa...	13A052	1
Hedinger	Fatty ointment anhydrous, wa...	13A053	1
Cordes	Fatty ointment anhydrous, wa...	13A052	1

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Supplier	Substance	Batch	Spectra
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	13A054	1
Gehe	Fatty ointment anhydrous, wa...	13A054	1
Ichtyol/Noweda	Fatty ointment anhydrous, wa...	13A053	1
Ichtyol-Gesellschaft	Fatty ointment anhydrous, wa...	13A053	1
Ichthyol-Gesellschaft/P...	Fatty ointment anhydrous, wa...	13A053	1
Ichthyol	Fatty ointment anhydrous, wa...	13A053	1
Ichthyol/Otto	Fatty ointment anhydrous, wa...	13A055	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	13A055	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	13A054	1
Ichthyol	Fatty ointment anhydrous, wa...	13A055	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A055	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	13A055	1
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	13A054	1
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	13A067	1
Ichtyol	Fatty ointment anhydrous, wa...	13A067	1
phönix/Ichthyol-Gesells...	Fatty ointment anhydrous, wa...	13A055	1
ichthyol gesellschaft	Fatty ointment anhydrous, wa...	13A055	1
Ichthyol	Fatty ointment anhydrous, wa...	13A067	1
Ichthyol	Fatty ointment anhydrous, wa...	13A068	2
Gehe/Ichthyol	Fatty ointment anhydrous, wa...	13A068	1
Euro OTC	Fatty ointment anhydrous, wa...	13A068	1
Ichthyol Gesellschaft/G...	Fatty ointment anhydrous, wa...	13A089	1
Cordes	Fatty ointment anhydrous, wa...	13A106	1
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	13A090	2
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	13A106	1
Gehe	Fatty ointment anhydrous, wa...	13A106	1
Ichthyol	Fatty ointment anhydrous, wa...	13A106	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	13A106	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	13A106	1
Ichthyol	Fatty ointment anhydrous, wa...	13A107	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	13A109	1
Ichthyol	Fatty ointment anhydrous, wa...	13A107	1
ichthyol/Gehe	Fatty ointment anhydrous, wa...	13A109	1
Ichthyol	Fatty ointment anhydrous, wa...	13A111	1
Ichtyol	Fatty ointment anhydrous, wa...	13A111	1
Ichthyol	Fatty ointment anhydrous, wa...	13A112	2
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	13A135	1
Ichtyol/ Phönix	Fatty ointment anhydrous, wa...	13A135	1
Gehe	Fatty ointment anhydrous, wa...	13A136	2
ICHTHYOL	Fatty ointment anhydrous, wa...	13A135	1
Ichthyol	Fatty ointment anhydrous, wa...	13A136	1
Ichthyol/Otto	Fatty ointment anhydrous, wa...	13A136	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	13A137	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	13A138	1
Caelo	Fatty ointment anhydrous, wa...	13A138	1
Gehe	Fatty ointment anhydrous, wa...	13A141	1
Stumpf/Ichtyol	Fatty ointment anhydrous, wa...	13A142	1
Gehe	Fatty ointment anhydrous, wa...	13A153	1
Caelo	Fatty ointment anhydrous, wa...	13A153	1
Ichthyol/Krieger/23.05...	Fatty ointment anhydrous, wa...	13A209	1
Stumpf/Ichtyol	Fatty ointment anhydrous, wa...	13A166	1
noweda/Ichtyol	Fatty ointment anhydrous, wa...	13A043	1
Caelo	Fatty ointment anhydrous, wa...	13A047	1
Ichtyol,Noweda	Fatty ointment anhydrous, wa...	13A047	1
ichthyol	Fatty ointment anhydrous, wa...	1413M-02532	1
Ichthyol/Sanacorp	Fatty ointment anhydrous, wa...	14A060	1
Ichtyol	Fatty ointment anhydrous, wa...	13A054	1
ichthyol gesellschaft	Fatty ointment anhydrous, wa...	15A022	1
ichthyol gesellschaft	Fatty ointment anhydrous, wa...	15A159	2
ichthyol gesellschaft	Fatty ointment anhydrous, wa...	15A041	1

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Supplier	Substance	Batch	Spectra
ichthyol gesellschaft	Fatty ointment anhydrous, wa...	16A011	1
Cordes	Fatty ointment anhydrous, wa...	15A060	1
Ichthyol	Fatty ointment anhydrous, wa...	15A123	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	16A073	1
ichtyol	Fatty ointment anhydrous, wa...	15a195	1
ichthyol gesellschaft	Fatty ointment anhydrous, wa...	15A076	1
ichthyol gesellschaft	Fatty ointment anhydrous, wa...	14A143	1
Ichtyol/Phönix	Fatty ointment anhydrous, wa...	4113Q-02532	1
Sanacorp	Fatty ointment anhydrous, wa...	2/AKD2	1
Caelo	Fatty ointment anhydrous, wa...	3112A-02532	1
Caelo	Fatty ointment anhydrous, wa...	Ichtyol	1
ichthyol	Fatty ointment anhydrous, wa...	20201112-1	1
Ichthyol	Fatty ointment anhydrous, wa...	11A202	2
Gehe/Apomix	Eye ointment, emulsifying DAC	1C080114	1
Apomix	Eye ointment, emulsifying DAC	1D040116	1
Apomix/Kehr	Eye ointment, emulsifying DAC	2D040116	1
Apomix / Kehr	Eye ointment, emulsifying DAC	48200114	1
Apomix / Sanacorp	Eye ointment, emulsifying DAC	4B200114	1
Noweda/apomix	Eye ointment, emulsifying DAC	4B200114	1
Caelo	Eye ointment, emulsifying DAC	5D110416	1
Apomix / Noweda	Eye ointment, emulsifying DAC	6A090516	1
Apomix/Kehr	Eye ointment, emulsifying DAC	7A160315	1
Apomix/Noweda	Eye ointment, emulsifying DAC	8D020414	1
Caelo	Emulsifying hydrophobic base...	13295801	3
Apomix / Noweda	Eye ointment, emulsifying DAC	9A080415	1
apomix/Sanacorp	Eye ointment, emulsifying DAC	9A190514	1
Caelo	Emulsifying hydrophobic base...	14087501	6
Caelo	Emulsifying hydrophobic base...	13340814	1
Caelo	Emulsifying hydrophobic base...	14276301	3
Caelo	Emulsifying hydrophobic base...	14161501	9
Caelo	Emulsifying hydrophobic base...	13361004	9
Caelo	Emulsifying hydrophobic base...	14276401	9
Caesar & Loretz GmbH	Emulsifying hydrophobic base...	14276401	2
Noweda	Emulsifying hydrophobic base...	14276401	2
Apomix / Kehr	Eye ointment, emulsifying DAC	14A011013	1
Apomix	Eye ointment, emulsifying DAC	14C170914	1
Phönix Gotha	Emulsifying hydrophobic base...	15064101	1
Caelo	Emulsifying hydrophobic base...	15064101	10
Caelo	Emulsifying hydrophobic base...	15205002	9
Caelo	Emulsifying hydrophobic base...	15269201	7
Caelo	Emulsifying hydrophobic base...	15331101	1
Caelo	Emulsifying hydrophobic base...	16054201	5
Caelo	Emulsifying hydrophobic base...	16054302	4
Caelo	Emulsifying hydrophobic base...	16172201	2
Caelo	Emulsifying hydrophobic base...	16172301	3
Apomix/Kehr	Eye ointment, emulsifying DAC	20D011215	1
apomix/Noweda	Eye ointment, emulsifying DAC	18C021115	1
PKH/Gehe	Eye ointment, emulsifying DAC	3B180213	2
Apomix/Noweda	Eye ointment, emulsifying DAC	7D210513	1
Noweda/apomix	Eye ointment, emulsifying DAC	18C021214	1
Apomix / Sanacorp	Eye ointment, emulsifying DAC	18C021214	1
Caelo	Eye ointment, emulsifying DAC	4A270212	1
PKH Halle / Noweda	Eye ointment, emulsifying DAC	9C250612	1
PKH/Gehe	Eye ointment, emulsifying DAC	10C170613	1
Apomix / AHD	Eye ointment, emulsifying DAC	11B170713	1
Apomix	Eye ointment, emulsifying DAC	7C040612	1
Apomix / Sanacorp	Eye ointment, emulsifying DAC	12C011012	1
apomix/ Sanacorp	Eye ointment, emulsifying DAC	12C300813	1
Noweda/ PKH Halle	Eye ointment, emulsifying DAC	16A061212	1
Apomix/Anzag	Eye ointment, emulsifying DAC	16B061212	1

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Supplier	Substance	Batch	Spectra
Gehe 07.03.13	Emulsifying hydrophobic base...	271904	2
Caelo	Emulsifying hydrophobic base...	12229003	4
Caelo	Emulsifying hydrophobic base...	12182301	1
Caelo	Emulsifying hydrophobic base...	12343501	6
Caelo	Emulsifying hydrophobic base...	13066802	10
gehe 13.07.2013	Emulsifying hydrophobic base...	13066802	2
Phönix 25.09.13	Emulsifying hydrophobic base...	13165201	1
Phoenix 05.11.2013	Emulsifying hydrophobic base...	13165205	1
Caelo	Emulsifying hydrophobic base...	13177601	7
Caelo	Emulsifying hydrophobic base...	13295701	8
Caelo	Emulsifying hydrophobic base...	20081302	1
Bombastus	Emulsifying hydrophobic base...	22011402	1
Bombastus	Emulsifying hydrophobic base...	279074	1
Bombastus	Wool alcohol ointment DAB	915M-01370	1
Caelo	Wool alcohol ointment DAB	14282901	2
Caelo	Wool alcohol ointment DAB	15361801	6
Caelo	Wool alcohol ointment DAB	15035503	2
Caelo	Wool alcohol ointment DAB	16007201	2
Caesar & Loretz/Noweda	Wool alcohol ointment DAB	16066601	1
Bombastus	Wool alcohol ointment DAB	293093	4
Sanacorp	Wool alcohol ointment DAB		1
Bombastus	Wool alcohol ointment DAB	298579	2
EuroOTV	Wool alcohol ointment DAB	1608040-01	1
Infectopharm/ Sanacorp	Wool alcohol ointment DAB	50334610	1
Beiersdorf / Phoenix	Wool alcohol ointment DAB	50845210	1
Beiersdorf AG/NOWEDA	Wool alcohol ointment DAB	50845210	1
Beiersdorf/Holdermann	Wool alcohol ointment DAB	50845210	1
Beiersdorf AG/Sanacorp	Wool alcohol ointment DAB	50444710	1
Beiersdorf/N	Wool alcohol ointment DAB	50925410	1
Beiersdorf	Wool alcohol ointment DAB	50925410	3
Beiersdorf	Wool alcohol ointment DAB	50935410	2
Beiersdorf / Noweda	Wool alcohol ointment DAB	50925410	1
Beiersdorf/Phönix	Wool alcohol ointment DAB	51015610	1
Beiersdorf /Sanacorp	Wool alcohol ointment DAB	51025610	1
Schärer & Schläpfer AG/...	Wool alcohol ointment DAB	50955510	1
Beiersdorf AG	Wool alcohol ointment DAB	51025610	1
Beiersdorf / Noweda	Wool alcohol ointment DAB	51115710	2
Beiersdorf	Wool alcohol ointment DAB	51946010	1
Beiersdorf/Phoenix	Wool alcohol ointment DAB	52656810	1
Beiersdorf direkt	Wool alcohol ointment DAB	52056110	1
Caelo	Wool alcohol ointment DAB	53437010	1
Beiersdorf	Wool alcohol ointment DAB	53437010	2
Beiersdorf/N	Wool alcohol ointment DAB	53437010	1
Beiersdorf/Noweda	Wool alcohol ointment DAB	53437010	1
Beiersdorf/Sanacorp	Wool alcohol ointment DAB	53437010	1
Beiersdorf/Gehe	Wool alcohol ointment DAB	53447010	1
Caelo	Wool alcohol ointment DAB	53457110	1
Beiersdorf /Alliance He...	Wool alcohol ointment DAB	54127710	1
Beiersdorf/Sana	Wool alcohol ointment DAB	54137710	1
Beiersdorf/N	Wool alcohol ointment DAB	53457110	1
Beiersdorf / Noweda	Wool alcohol ointment DAB	54147810	1
Beiersdorf/N	Wool alcohol ointment DAB	60839310	1
Beiersdorf/Noweda	Wool alcohol ointment DAB	54147810	1
Beiersdorf	Wool alcohol ointment DAB	61079710	1
Beiersdorf	Wool alcohol ointment DAB	54127710	1
Beiersdorf	Wool alcohol ointment DAB	60419110	1
Beiersdorf / Phoenix	Wool alcohol ointment DAB	62031710	1
Beiersdorf/N	Wool alcohol ointment DAB	54147810	1
Beiersdorf	Wool alcohol ointment DAB	54157810	1
Ebert 18.10.16	Wool alcohol ointment DAB	62031710	1

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Supplier	Substance	Batch	Spectra
Beiersdorf / Noweda	Wool alcohol ointment DAB	54157810	1
Beiersdorf/AHC	Wool alcohol ointment DAB	62932210	1
Beiersdorf / Kehr	Wool alcohol ointment DAB	61149910	1
Bombastus	Wool alcohol ointment DAB	1211018-01	1
Caelo	Wool alcohol ointment DAB	131255101	1
Caelo	Wool alcohol ointment DAB	13255001	9
Sanacorp	Wool alcohol ointment DAB	13255001	1
Caelo	Wool alcohol ointment DAB	13242602	10
Caelo	Wool alcohol ointment DAB	13242601	10
Caelo	Wool alcohol ointment DAB	13255101	22
Caelo	Wool alcohol ointment DAB	14067002	6
Caelo	Wool alcohol ointment DAB	13255201	9
Caelo	Wool alcohol ointment DAB	14067201	8
Caelo	Wool alcohol ointment DAB	14153101	11
Caelo	Wool alcohol ointment DAB	14153602	2
Caelo	Wool alcohol ointment DAB	14153603	8
Bombastus	Wool alcohol ointment DAB	289510	3
Caelo	Wool alcohol ointment DAB	15034801	3
Bombastus	Wool alcohol ointment DAB	279927	3
Caelo	Wool alcohol ointment DAB	14283101	2
Caelo	Wool alcohol ointment DAB	15034901	5
Phönix Gotha	Wool alcohol ointment DAB	14282801	1
Caelo	Wool alcohol ointment DAB	14282801	6
Beiersdorf AG	Wool alcohol ointment DAB	33753710	1
Beiersdorf	Wool alcohol ointment DAB	34554710	4
Beiersdorf/Phönix	Wool alcohol ointment DAB	34554710	1
Beiersdorf AG	Wool alcohol ointment DAB	40956810	1
Beiersdorf	Wool alcohol ointment DAB	40956810	2
Beiersdorf	Wool alcohol ointment DAB	40726610	1
Stumpf/Beiersdorf Ag	Wool alcohol ointment DAB	40956810	1
Großhandel	Wool alcohol ointment DAB	40956810	1
Anzag/Beiersdorf	Wool alcohol ointment DAB	40930610	1
Beiersdorf / Sanacorp	Wool alcohol ointment DAB	41026910	1
Caelo	Wool alcohol ointment DAB	41026910	1
Gehe	Wool alcohol ointment DAB	41026910	1
Beiersdorf AG / Phönix	Wool alcohol ointment DAB	40956810	1
Beiersdorf	Wool alcohol ointment DAB	41026910	1
Beiersdorf/Kehr	Wool alcohol ointment DAB	4104701008/16	1
Sanacorp	Wool alcohol ointment DAB	41047010	1
Beiersdorf/Otto	Wool alcohol ointment DAB	41047010	1
Beiersdorf	Wool alcohol ointment DAB	41839810	2
Beiersdorf AG	Wool alcohol ointment DAB	41829810	1
Beiersdorf/Noweda	Wool alcohol ointment DAB	41910710	1
Stumpf/Beiersdorf Ag	Wool alcohol ointment DAB	41910710	1
Beiersdorf/Phoenix	Wool alcohol ointment DAB	41910710	1
Noweda / Beiersdorf AG	Wool alcohol ointment DAB	41930610	1
Beiersdorf/ Gehe	Wool alcohol ointment DAB	41930610	1
Beiersdorf/Gehe	Wool alcohol ointment DAB	41930610	1
Beiersdorf AG / Phönix	Wool alcohol ointment DAB	41940610	1
Beiersdorf/Phoenix	Wool alcohol ointment DAB	41930610	1
Beiersdorf	Wool alcohol ointment DAB	41940610	1
Beiersdorf/ Gehe	Wool alcohol ointment DAB	41950710	1
Beiersdorf	Wool alcohol ointment DAB	42531910	1
Beiersdorf SA	Wool alcohol ointment DAB	41950710	1
Sanacorp	Wool alcohol ointment DAB	43112910	1
Gehe	Wool alcohol ointment DAB	43142910	1
Beiersdorf/ Noweda	Wool alcohol ointment DAB	43142910	1
Gehe	Wool alcohol ointment DAB	45054410	1
Beiersdorf SA	Wool alcohol ointment DAB	44824310	1
Noweda / Beiersdorf AG	Wool alcohol ointment DAB	45054410	1

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Supplier	Substance	Batch	Spectra
Beiersdorf/Noweda	Wool alcohol ointment DAB	45054410	2
Caelo	Wool alcohol ointment DAB	46/AKD2	1
Caelo	Wool alcohol ointment DAB	50414810	1
Beiersdorf	Wool alcohol ointment DAB	50324610	1
Noweda/Beiersdorf	Wool alcohol ointment DAB	50324610	1
Beiersdorf/Noweda	Wool alcohol ointment DAB	50324610	1
Beiersdorf über Sanacorp	Wool alcohol ointment DAB	50444710	1
Gehe/Beiersdorf	Wool alcohol ointment DAB	50414810	1
Beiersdorf	Wool alcohol ointment DAB	50444710	4
Baiersdorf	Wool alcohol ointment DAB	4833010	1
Noweda / Beiersdorf AG	Wool alcohol ointment DAB	50815310	1
Beiersdorf AG/Noweda	Wool alcohol ointment DAB	50815310	1
Caelo	Wool alcohol ointment DAB		9
Caelo	Wool alcohol ointment DAB	1212M-01370	1
Sanacorp	Wool alcohol ointment DAB	12151801	1
Bombastus	Wool alcohol ointment DAB	1109210014	1
Fagron	Wool alcohol ointment DAB	1234	2
Caelo	Wool alcohol ointment DAB	12152001	5
Caelo	Wool alcohol ointment DAB	13067102	12
Caelo	Wool alcohol ointment DAB	13114001	7
Caelo	Wool alcohol ointment DAB	13114102	7
Phönix	Wool alcohol ointment DAB	13114103	1
Caelo	Wool alcohol ointment DAB	13126102	1
Caelo	Wool alcohol ointment DAB	13242901	5
Gehe	Wool alcohol ointment DAB	13357910	1
Beiersdorf (DAB 2010)	Wool alcohol ointment DAB	13658410	1
Beiersdorf	Wool alcohol ointment DAB	14021301	1
Caelo	Wool alcohol ointment DAB	14024701	1
Gehe	Wool alcohol ointment DAB	21241410	2
Beiersdorf	Wool alcohol ointment DAB	14939610	1
Beiersdorf	Wool alcohol ointment DAB	20440810	1
Gehe	Wool alcohol ointment DAB	22412510	2
Beiersdorf	Wool alcohol ointment DAB	21241410	1
Beiersdorf (DAB 2010)	Wool alcohol ointment DAB	22412510	1
Beiersdorf	Wool alcohol ointment DAB	22142410	1
Beiersdorf	Wool alcohol ointment DAB	21431810	1
Anzag	Wool alcohol ointment DAB	22412510	2
BDF Phönix	Wool alcohol ointment DAB	22422510	1
Noweda	Wool alcohol ointment DAB	22532710	1
Phoenix	Wool alcohol ointment DAB	22532710	1
Phönix/Beiersdorf	Wool alcohol ointment DAB	23023210	1
Caelo	Wool alcohol ointment DAB	2313E-01370	1
Caelo	Wool alcohol ointment DAB	23023210	2
Beiersdorf AG / Noweda	Wool alcohol ointment DAB	22532710	1
Beiersdorf	Wool alcohol ointment DAB	23223410	3
Stumpf	Wool alcohol ointment DAB	23223410	1
Anzag/	Wool alcohol ointment DAB	23223410	1
Beiersdorf AG	Wool alcohol ointment DAB	23223410	1
BDF	Wool alcohol ointment DAB	2322410	1
Beiersdorf	Wool alcohol ointment DAB	23753710	1
Gehe	Wool alcohol ointment DAB	23753710	1
Beiersdorf	Wool alcohol ointment DAB	24113810	1
Beiersdorf/Gehe	Wool alcohol ointment DAB	24123810	1
Beiersdorf	Wool alcohol ointment DAB	24233910	2
Beiersdorf / Noweda	Wool alcohol ointment DAB	24233910	1
Phönix/Beiersdorf	Wool alcohol ointment DAB	24243910	1
Anzag	Wool alcohol ointment DAB	24254010	1
Sanacorp	Wool alcohol ointment DAB	24254010	1
Beiersdorf AG	Wool alcohol ointment DAB	24254010	1
Beiersdorf AG	Wool alcohol ointment DAB	24635410	1

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Supplier	Substance	Batch	Spectra
Beiersdorf	Wool alcohol ointment DAB	24254010	1
Beiersdorf	Wool alcohol ointment DAB	24635410	4
Noweda	Wool alcohol ointment DAB	24635410	1
Bombastus	Wool alcohol ointment DAB	281690	3
Gehe	Wool alcohol ointment DAB	30711310	1
beiersdorf/Gehe	Wool alcohol ointment DAB	30721310	1
Beiersdorf S.A.	Wool alcohol ointment DAB	30731210	1
Caelo	Wool alcohol ointment DAB	30731210	1
Beiersdorf Manufacturing	Wool alcohol ointment DAB	30731210	1
Beiersdorf AG	Wool alcohol ointment DAB	30821610	1
Beiersdorf AG	Wool alcohol ointment DAB	30731210	2
Gehe	Wool alcohol ointment DAB	30831410	2
Beiersdorf	Wool alcohol ointment DAB	30831410	1
Beiersdorf AG/NOWEDA	Wool alcohol ointment DAB	30831410	1
Beiersdorf	Wool alcohol ointment DAB	30841410	4
Beiersdorf S.A.	Wool alcohol ointment DAB	30851510	1
Stumpf	Wool alcohol ointment DAB	30851510	1
Sanacorp	Wool alcohol ointment DAB	30851510	1
alliance Healthcare/Bei...	Wool alcohol ointment DAB	30851510	1
Caelo	Wool alcohol ointment DAB	30841410	1
Caelo	Wool alcohol ointment DAB	31121710	2
Gehe	Wool alcohol ointment DAB	30851510	1
Phönix	Wool alcohol ointment DAB	31322010	1
Beiersdorf AG	Wool alcohol ointment DAB	31231810	2
Beiersdorf/Sanacorp	Wool alcohol ointment DAB	31231810	1
Beiersdorf/Otto	Wool alcohol ointment DAB	31251910	1
Gehe	Wool alcohol ointment DAB	31231810	1
Beiersdorf/Noweda	Wool alcohol ointment DAB	31322010	2
Stumpf/Beiersdorf Ag	Wool alcohol ointment DAB	33323210	1
Beiersdorf/ Noweda	Wool alcohol ointment DAB	33323210	2
Beiersdorf S.A.	Wool alcohol ointment DAB	32352710	1
Beiersdorf	Wool alcohol ointment DAB	33323210	2
Gehe	Wool alcohol ointment DAB	33323210	1
Beiersdorf/Krieger/06.1...	Wool alcohol ointment DAB	33323210	1
Beiersdorf AG/Noweda	Wool alcohol ointment DAB	33323210	2
Beiersdorf/Gumo	Wool alcohol ointment DAB	33323210	1
Beiersdorf	Wool alcohol ointment DAB	33343310	2
BDF	Wool alcohol ointment DAB	33343310	1
Beiersdorf AG	Wool alcohol ointment DAB	33343310	1
Stumpf/Beiersdorf Ag	Wool alcohol ointment DAB	33343310	1
Beiersdorf/Phönix	Wool alcohol ointment DAB	33343310	1
Beiersdorf	Wool alcohol ointment DAB	33723610	2
Beiersdorf/V.d.L.	Wool alcohol ointment DAB	33723610	1
Beiersdorf/Phönix	Wool alcohol ointment DAB	33723610	1
Sanacorp/ Beiersdorf	Wool alcohol ointment DAB	33723610	1
Caelo	Wool alcohol ointment DAB	33753710	1
Gehe	Wool alcohol ointment DAB	33753710	3
Beiersdorf/Otto	Wool alcohol ointment DAB	33753710	1
Beiersdorf	Wool alcohol ointment DAB	34224110	1
Beiersdorf / Noweda	Wool alcohol ointment DAB	34414610	2
Beiersdorf/Sanacorp	Wool alcohol ointment DAB	34254110	1
Beiersdorf S.A.	Wool alcohol ointment DAB	34414610	1
Beiersdorf	Wool alcohol ointment DAB	34414610	1
Beiersdorf/Noweda	Wool alcohol ointment DAB	34424610	1
Beiersdorf	Wool alcohol ointment DAB	41047010	1
Beiersdorf	Wool alcohol ointment DAB	50845210	1
Beiersdorf AG/ GEHE	Wool alcohol ointment DAB	41829810	1
Beiersdorf	Wool alcohol ointment DAB	50414810	1
Ichthyol -Gesellschaft	Fatty ointment anhydrous, wa...	13A091	1
ichthyol	Fatty ointment anhydrous, wa...	13A090	1

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Supplier	Substance	Batch	Spectra
Ichthyol / Phoenix	Fatty ointment anhydrous, wa...	13A091	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	13A159	1
Cordes, Hermani / Gehe	Fatty ointment anhydrous, wa...	14A112	1
Ichthyol/AHP	Fatty ointment anhydrous, wa...	154141	1
Noweda/Ichthyol	Fatty ointment anhydrous, wa...	15A020	2
Noweda/Ichthyol	Fatty ointment anhydrous, wa...	14A173	1
Caelo	Fatty ointment anhydrous, wa...	13A181	1
Ichthyol	Fatty ointment anhydrous, wa...	14A116	1
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	15A011	1
Ichthyol	Fatty ointment anhydrous, wa...	15A021	1
Alliance health	Fatty ointment anhydrous, wa...	15A023	1
Ichthyol Gesellschaft Co...	Fatty ointment anhydrous, wa...	15A021	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	15A023	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	15A023	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	15A021	1
Ichthyol-Gesellschaft C...	Fatty ointment anhydrous, wa...	15A023	1
Phoenix	Fatty ointment anhydrous, wa...	15A027	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	15A027	1
Ichthyol-Gesellschaft/Sa...	Fatty ointment anhydrous, wa...	15A037	1
Noweda / Ichthyol Gesel...	Fatty ointment anhydrous, wa...	15A060	1
Ichthyol/Sanova Pharma	Fatty ointment anhydrous, wa...	15A041	1
Ichthyol Gesellschaft/S...	Fatty ointment anhydrous, wa...	15A060	2
Ichthyol	Fatty ointment anhydrous, wa...	15A060	2
ICHTHYOL-GESELLSCHAFT C...	Fatty ointment anhydrous, wa...	15A060	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	15A060	1
Caelo	Fatty ointment anhydrous, wa...	15A061	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	15A061	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	15A061	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	15A062	2
Ichthyol-Gesellschaft C...	Fatty ointment anhydrous, wa...	15A062	1
Ichthyol / Sanacorp	Fatty ointment anhydrous, wa...	15A062	1
Ichthyol /Noweda	Fatty ointment anhydrous, wa...	15a073	1
Ichthyol / Noweda	Fatty ointment anhydrous, wa...	15A073	1
Ichthyol	Fatty ointment anhydrous, wa...	15A074	1
Stumpf/Ichthyol-Gesells...	Fatty ointment anhydrous, wa...	15A089	1
Ichthyol/AHC	Fatty ointment anhydrous, wa...	15A089	1
Ichthyol	Fatty ointment anhydrous, wa...	15A089	1
Ichthyol Gesellschaft/ ...	Fatty ointment anhydrous, wa...	15A090	1
Ichthyol	Fatty ointment anhydrous, wa...	15A092	1
Ichthyol über Phoenix	Fatty ointment anhydrous, wa...	15A092	1
Caelo	Fatty ointment anhydrous, wa...	15A106	1
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	15A106	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	15A124	1
Phönix/Ichthyol	Fatty ointment anhydrous, wa...	15A123	1
Noweda/Ichthyol-Gesells...	Fatty ointment anhydrous, wa...	15A123	1
Ichthyol/Sanacorp	Fatty ointment anhydrous, wa...	15A106	1
Noweda/Ichthyol	Fatty ointment anhydrous, wa...	15A123	1
Ichthyol/Noweda	Fatty ointment anhydrous, wa...	15A124	1
Cordes/Phönix	Fatty ointment anhydrous, wa...	15A124	1
Ichthyol Gesellschaft /...	Fatty ointment anhydrous, wa...	15A125	1
Ichthyol	Fatty ointment anhydrous, wa...	15A137	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	15A125	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	15A137	1
Ichthyol	Fatty ointment anhydrous, wa...	15A140	1
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	15A141	1
Ichthyol über Phoenix	Fatty ointment anhydrous, wa...	15A142	1
Ichthyol	Fatty ointment anhydrous, wa...	15A148	2
Phoenix	Fatty ointment anhydrous, wa...	15A149	1
Caelo	Fatty ointment anhydrous, wa...	15A149	1
Bombastus	Fatty ointment anhydrous, wa...	15A149	1

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Supplier	Substance	Batch	Spectra
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	15A156	1
Caelo	Fatty ointment anhydrous, wa...	15A150	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	15A156	1
Caelo	Fatty ointment anhydrous, wa...	15A159	1
Ichthyol / Gehe	Fatty ointment anhydrous, wa...	15A162	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	15A191	1
Caelo	Fatty ointment anhydrous, wa...	15A192	1
Ichthyol/Phoenix	Fatty ointment anhydrous, wa...	15A191	1
Noweda	Fatty ointment anhydrous, wa...	15A192	1
Gehe/Ichthyol	Fatty ointment anhydrous, wa...	15A191	1
Ichthyol über Phoenix	Fatty ointment anhydrous, wa...	16A044	1
Ichthyol-Gesellschaft/ ...	Fatty ointment anhydrous, wa...	16A013	1
Phoenix	Fatty ointment anhydrous, wa...	16A045	1
Ichthyol/N	Fatty ointment anhydrous, wa...	16A046	1
Phoenix	Fatty ointment anhydrous, wa...	16A046	1
Ebert 17.08.16 KKH	Fatty ointment anhydrous, wa...	16A048	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	16A083	1
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	16A083	1
Caelo	Fatty ointment anhydrous, wa...	16A044	1
Ichthyol	Fatty ointment anhydrous, wa...	16A123	1
PHÖNIX	Fatty ointment anhydrous, wa...	16A124	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	16A083	1
Ichthyol	Fatty ointment anhydrous, wa...	16A124	1
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	1713M-02532	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	31072015A	1
Ichthyol/Alliance Healt...	Fatty ointment anhydrous, wa...	16A099	1
ichthyol	Fatty ointment anhydrous, wa...		1
Fagron	Fatty ointment anhydrous, wa...	Ichthyol/Phoenix	1
ICHTHYOL-GES/GEHE	Fatty ointment anhydrous, wa...	11A040	1
Ichthyol	Fatty ointment anhydrous, wa...	11A042	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	10A026	1
ICHTHYOL-GES/GEHE	Fatty ointment anhydrous, wa...	10A016	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	11A085	1
Ichthyol	Fatty ointment anhydrous, wa...	11A043	1
Ichthyol/Gehe	Fatty ointment anhydrous, wa...	11A043	1
Ichthyol-Gesellschaft, ...	Fatty ointment anhydrous, wa...	11A122	1
Ichthyol	Fatty ointment anhydrous, wa...	11A120	1
Caelo	Fatty ointment anhydrous, wa...	11A146	1
Ichthyol/Krieger	Fatty ointment anhydrous, wa...	11A146	1
Ichthyol	Fatty ointment anhydrous, wa...	11A150	1
Caelo	Fatty ointment anhydrous, wa...	11A162	1
Ichthyol-Gesellschaft, ...	Fatty ointment anhydrous, wa...	11A162	1
Ichthyol	Fatty ointment anhydrous, wa...	11A153	1
Ichthyol	Fatty ointment anhydrous, wa...	11A187	2
Sanacorp/ Sanova	Fatty ointment anhydrous, wa...	11A187	1
Noweda	Fatty ointment anhydrous, wa...	11a199	1
Caelo	Fatty ointment anhydrous, wa...	11A202	1
Ichthyol/Krieger	Fatty ointment anhydrous, wa...	11A202	1
Hersteller: Ichthyol	Fatty ointment anhydrous, wa...	11A202	1
ichthyol- gesellschaft ...	Fatty ointment anhydrous, wa...	11A202	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	11A234	1
Anzag 26.09.2012	Fatty ointment anhydrous, wa...	11A202	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	11A202	1
Caelo	Fatty ointment anhydrous, wa...	12A056	1
Gehe	Fatty ointment anhydrous, wa...	11A234	1
Anzag 29.10.12	Fatty ointment anhydrous, wa...	12A007	1
ichthyol	Fatty ointment anhydrous, wa...	12A129	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	12A041	1
Caelo	Fatty ointment anhydrous, wa...	12A021	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	11A233	1

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Supplier	Substance	Batch	Spectra
Ichthyol	Fatty ointment anhydrous, wa...	12A053	2
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	12A053	1
Anzag	Fatty ointment anhydrous, wa...	12A055	1
Gehe	Fatty ointment anhydrous, wa...	12A056	2
Ichthyol/ Noweda	Fatty ointment anhydrous, wa...	12A053	1
Gehe	Fatty ointment anhydrous, wa...	12A054	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	12A058	1
Caelo	Fatty ointment anhydrous, wa...	12A060	1
Ichthyol Cordes	Fatty ointment anhydrous, wa...	12A075	2
Ichthyol	Fatty ointment anhydrous, wa...	12A064	1
Gehe	Fatty ointment anhydrous, wa...	12A075	1
Ichthyol -Gesellschaft	Fatty ointment anhydrous, wa...	12A064	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	12A077	1
ichthyol	Fatty ointment anhydrous, wa...	12A060	1
Caelo	Fatty ointment anhydrous, wa...	12A078	1
phönix/Ichthyol-Gesells...	Fatty ointment anhydrous, wa...	12A078	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	12A079	1
Gehe	Fatty ointment anhydrous, wa...	12A079	1
Phoenix	Fatty ointment anhydrous, wa...	12A087	1
Gehe	Fatty ointment anhydrous, wa...	12A087	1
Hersteller: Ichthyol/Gehe	Fatty ointment anhydrous, wa...	12A102	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	12A087	1
ichthyol	Fatty ointment anhydrous, wa...	12A102	1
Fagron	Fatty ointment anhydrous, wa...	12A115	1
Stumpf/Ichthyol	Fatty ointment anhydrous, wa...	12A115	1
Ichthyol	Fatty ointment anhydrous, wa...	12A120	1
Ichthyol	Fatty ointment anhydrous, wa...	12A123	1
Gehe	Fatty ointment anhydrous, wa...	12A124	1
Phönix	Fatty ointment anhydrous, wa...	12A129	1
ichthyol,Anzag	Fatty ointment anhydrous, wa...	12A124	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	12A129	1
Ichthyl Phönix	Fatty ointment anhydrous, wa...	12A129	1
Caelo	Fatty ointment anhydrous, wa...	12A130	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	12A130	1
Caelo	Fatty ointment anhydrous, wa...	12a123	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	12A130	1
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	12A124	1
Ichthyol	Fatty ointment anhydrous, wa...	12A139	1
Ichthyol,Noweda	Fatty ointment anhydrous, wa...	12A139	1
Caelo	Fatty ointment anhydrous, wa...	12A131	1
Großhandel	Fatty ointment anhydrous, wa...	12A140	1
Ichthyol,Noweda	Fatty ointment anhydrous, wa...	12A142	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	12A156	1
Ichthyol	Fatty ointment anhydrous, wa...	12A157	1
Noweda	Fatty ointment anhydrous, wa...	12A184	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	12A206	1
Ichthyol-Gesellschaft C...	Fatty ointment anhydrous, wa...	12A184	1
Alliance	Fatty ointment anhydrous, wa...	12A184	1
Gehe	Fatty ointment anhydrous, wa...	12A211	1
Ichthyol/14.01.14/K	Fatty ointment anhydrous, wa...	13A026	1
Phoenix/Ichthyol	Fatty ointment anhydrous, wa...	13A055	1
Ichthyol Gesellschaft C...	Fatty ointment anhydrous, wa...	13A031	1
ichthyol	Fatty ointment anhydrous, wa...	13A1008	1
Ichthyol	Fatty ointment anhydrous, wa...	26101201	1
Ichthiol	Fatty ointment anhydrous, wa...	2112212532	1
Ichthyol	Fatty ointment anhydrous, wa...	14121203	1
Caelo	Hydrophobic base gel DAC	14102505	2
Caelo	Emulsifying hydrophobic base...	12362505	2
Sanacorp	Hydrophobic base gel DAC	13165201	1
Bombastus	Emulsifying hydrophobic base...	282094	1

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Supplier	Substance	Batch	Spectra
Eigen Defektur	Hydrophilic ointment DAB	316M-02539	1
Caelo	Hydrophilic ointment DAB	1120462	1
Caelo	Hydrophilic ointment DAB	916I-02539	1
Caelo	Hydrophilic ointment DAB	12051401	1
Caelo	Hydrophilic ointment DAB	13117501	11
Caesar&Loretz GmbH/Anzag	Hydrophilic ointment DAB	13245301	1
Caelo	Hydrophilic ointment DAB	13245401	9
Caelo	Hydrophilic ointment DAB	13245601	7
Caelo	Hydrophilic ointment DAB	13245301	7
Caelo	Hydrophilic ointment DAB	13245501	6
Großhandel	Hydrophilic ointment DAB	13245701	1
Caelo	Hydrophilic ointment DAB	13245701	5
Caelo	Hydrophilic ointment DAB	13245901	9
Fagron	Hydrophilic ointment DAB	13H13T04006144	1
Caelo	Hydrophilic ointment DAB	14024601	3
Alliance Health 09.05.2...	Hydrophilic ointment DAB	14024701	1
Caelo	Hydrophilic ointment DAB	14024701	11
Caelo	Hydrophilic ointment DAB	14024803	4
Phönix	Hydrophilic ointment DAB	14024701	1
Caelo	Hydrophilic ointment DAB	14024802	4
Caesar & Loretz GmbH	Hydrophilic ointment DAB	14024901	2
Caelo	Hydrophilic ointment DAB	14024901	5
Caelo	Hydrophilic ointment DAB	14025001	9
Caelo	Hydrophilic ointment DAB	14123101	7
Caelo	Hydrophilic ointment DAB	14123301	7
Caelo	Hydrophilic ointment DAB	14123201	3
Caelo	Hydrophilic ointment DAB	14123401	8
Caelo	Hydrophilic ointment DAB	14123502	2
Caelo	Hydrophilic ointment DAB	14224701	2
Caelo	Hydrophilic ointment DAB	14224901	4
Caelo	Hydrophilic ointment DAB	14225001	7
Caelo	Hydrophilic ointment DAB	14225002	9
Caelo	Hydrophilic ointment DAB	14231901	5
Caelo	Hydrophilic ointment DAB	1423101	1
Caelo	Hydrophilic ointment DAB	14277601	6
Caelo	Hydrophilic ointment DAB	14277701	2
Caesar & Loretz GmbH	Hydrophilic ointment DAB	14277801	1
Caelo	Hydrophilic ointment DAB	14277801	4
Caelo	Hydrophilic ointment DAB	14277901	10
Caesar&Loretz GmbH/Anzag	Hydrophilic ointment DAB	14277901	1
Caesar & Loretz GmbH	Hydrophilic ointment DAB	14277901	1
Caelo	Hydrophilic ointment DAB	14278003	2
Fagron	Hydrophilic ointment DAB	14A06-T10-009049	1
Fagron	Hydrophilic ointment DAB	14A06-T11	1
Fagron	Hydrophilic ointment DAB	14A06-T11-009054	1
Euro OTC	Hydrophilic ointment DAB	14A06-T10-009049	1
Fagron	Hydrophilic ointment DAB	14A06T11009054	1
Fagron	Hydrophilic ointment DAB	14G08-T06	1
Fagron	Hydrophilic ointment DAB	14G08-T06-013947	2
Fagron	Hydrophilic ointment DAB	14G08-T06-013948	1
Fagron	Hydrophilic ointment DAB	14G08-T07-013951	1
Fagron	Hydrophilic ointment DAB	14G08-T08-013954	2
Caelo	Hydrophilic ointment DAB	15016502	5
Caelo	Hydrophilic ointment DAB	15016503	4
Caelo	Hydrophilic ointment DAB	15016601	7
Caelo	Hydrophilic ointment DAB	15016602	2
Caelo	Hydrophilic ointment DAB	15016701	3
Caelo	Hydrophilic ointment DAB	15016801	6
Caelo	Hydrophilic ointment DAB	15016901	7
Caelo	Hydrophilic ointment DAB	15097714	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrophilic ointment DAB	15113602	1
Caelo	Hydrophilic ointment DAB	15221601	6
Caelo	Hydrophilic ointment DAB	15221602	3
Caelo	Hydrophilic ointment DAB	15221701	12
Noweda 06.04.2016	Hydrophilic ointment DAB	15221601	1
Caesar & Loretz GmbH	Hydrophilic ointment DAB	15221701	2
Caelo	Hydrophilic ointment DAB	15221801	1
Caelo	Hydrophilic ointment DAB	15221901	1
Caelo	Hydrophilic ointment DAB	15400701	1
Caelo	Hydrophilic ointment DAB	15416401	9
Caelo	Hydrophilic ointment DAB	15416502	6
Fagron	Hydrophilic ointment DAB	15B19-T01-019409	1
Fagron	Hydrophilic ointment DAB	15B19-T01	1
Fagron	Hydrophilic ointment DAB	15F24-T05-023887	1
Fagron	Hydrophilic ointment DAB	15F09-T02-023370	1
Fagron	Hydrophilic ointment DAB	15B19-T01-019411	2
Fagron	Hydrophilic ointment DAB	15K24-T01-027590	1
Caesar & Loretz GmbH Hi...	Hydrophilic ointment DAB	16008701	2
Caelo	Hydrophilic ointment DAB	16008701	4
Ebert & Jacobi 03.08.16	Hydrophilic ointment DAB	160091001	1
Caelo	Hydrophilic ointment DAB	16008702	4
Caelo	Hydrophilic ointment DAB	16009101	7
Caesar&Loretz GmbH/Anzag	Hydrophilic ointment DAB	16009101	1
Caelo	Hydrophilic ointment DAB	16009201	3
Caelo	Hydrophilic ointment DAB	16009301	1
Anzag/Ichtyol-Gesellsch...	Hydrophilic ointment DAB	16009201	1
Caelo	Hydrophilic ointment DAB	1614U2539	1
Caelo	Hydrophilic ointment DAB	16166701	4
Caesar & Loretz	Hydrophilic ointment DAB	16166701	1
Caelo	Hydrophilic ointment DAB	16166902	2
Caelo	Hydrophilic ointment DAB	16166801	7
Caelo	Hydrophilic ointment DAB	16167001	1
Eigen Defektur	Hydrophilic ointment DAB	1716E-02539	1
Henry Lamotte/Anzag	Hydrophilic ointment DAB	2215M-02539	1
Eigen/Defektur	Hydrophilic ointment DAB	2516A-02539	1
Bombastus	Hydrophilic ointment DAB	281248	1
Bombastus	Hydrophilic ointment DAB	281346	2
Bombastus	Hydrophilic ointment DAB	281347	3
Bombastus	Hydrophilic ointment DAB	281348	3
Caelo	Hydrophilic ointment DAB	281349	2
Bombastus	Hydrophilic ointment DAB	281351	6
Bombastus	Hydrophilic ointment DAB	284748	2
Bombastus	Hydrophilic ointment DAB	284747	1
Bombastus	Hydrophilic ointment DAB	284746	1
Bombastus	Hydrophilic ointment DAB	286544	5
Caelo	Hydrophilic ointment DAB	286545	1
Bombastus	Hydrophilic ointment DAB	286545	3
Bombastus	Hydrophilic ointment DAB	288367	2
Bombastus	Hydrophilic ointment DAB	288366	1
Bombastus	Hydrophilic ointment DAB	288368	1
Bombastus	Hydrophilic ointment DAB	288369	2
Bombastus	Hydrophilic ointment DAB	290597	1
Bombastus	Hydrophilic ointment DAB	290599	3
Bombastus	Hydrophilic ointment DAB	290600	2
Bombastus	Hydrophilic ointment DAB	290601	3
Bombastus	Hydrophilic ointment DAB	293261	1
Bombastus	Hydrophilic ointment DAB	293262	3
Bombastus	Hydrophilic ointment DAB	293263	2
Bombastus	Hydrophilic ointment DAB	293264	2
Bombastus	Hydrophilic ointment DAB	294448	2

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Supplier	Substance	Batch	Spectra
Bombastus	Hydrophilic ointment DAB	294451	2
Caelo	Hydrophilic ointment DAB	294449	2
Bombastus	Hydrophilic ointment DAB	296865	2
Bombastus	Hydrophilic ointment DAB	296866	2
Bombastus	Hydrophilic ointment DAB	296867	1
Bombastus	Hydrophilic ointment DAB	296868	5
Defektur / Wolf-Apotheke	Hydrophilic ointment DAB	299390	3
Bombastus	Hydrophilic ointment DAB	299392	2
Bombastus	Hydrophilic ointment DAB	301097	1
Bombastus	Hydrophilic ointment DAB	301096	1
Eigen/Defektur	Hydrophilic ointment DAB	3415I-02539	1
Defekur	Hydrophilic ointment DAB	3216M-02539	1
Eigen/Defektur	Hydrophilic ointment DAB	4215E-02539	1
Eigen/Defektur	Hydrophilic ointment DAB	5015E-02539	1
lamotte	Hydrophilic ointment DAB	5448000	1
Lamotte/Alliance	Hydrophilic ointment DAB	5651600	1
lamotte	Hydrophilic ointment DAB	5517900	1
Lamotte//AHD	Hydrophilic ointment DAB	5860500	1
Fiebig/ Lamotte	Hydrophilic ointment DAB	5860400	1
Lamotte/ANZAG	Hydrophilic ointment DAB	5860400	1
Sanacorp	Hydrophilic ointment DAB		1
Caelo	Hydrophilic ointment DAB		4
Caelo	Hydrophilic ointment DAB	11133701	1
Caelo	Hydrophilic ointment DAB	11211601	2
Caelo	Hydrophilic ointment DAB	11212101	5
Caelo	Hydrophilic ointment DAB	11133502	1
Gehe	Hydrophilic ointment DAB	11L13-T01	2
Caelo	Hydrophilic ointment DAB	12014601	1
Caelo	Hydrophilic ointment DAB	11212201	2
Gehe	Hydrophilic ointment DAB	12014601	1
Caelo	Hydrophilic ointment DAB	12014602	3
Caelo	Hydrophilic ointment DAB	12014701	3
Caelo	Hydrophilic ointment DAB	2803212539	1
Caelo	Hydrophilic ointment DAB	12014801	1
Bombastus	Hydrophilic ointment DAB	269532	1
Bombastus	Hydrophilic ointment DAB	269537	1
Stumpf	Hydrophilic ointment DAB	269539	1
Bombastus	Hydrophilic ointment DAB	269536	1
Bombastus	Hydrophilic ointment DAB	269538	3
Bombastus	Hydrophilic ointment DAB	269539	2
Stumpf	Hydrophilic ointment DAB	274004	1
Caelo	Hydrophilic ointment DAB	70913UngEm	1
Caelo	Hydrophilic ointment DAB	11015402	1
Caelo	Hydrophilic ointment DAB	11133601	2
Caelo	Hydrophilic ointment DAB	10025601	1
Caelo	Hydrophilic ointment DAB	10082901	1
Euro OTC	Hydrophilic ointment DAB	11211601	2
Caelo	Hydrophilic ointment DAB	11335101	2
Caelo	Hydrophilic ointment DAB	103312539	1
Caelo	Hydrophilic ointment DAB	11212001	1
Noweda	Hydrophilic ointment DAB	12014601	1
Caelo	Hydrophilic ointment DAB	12015001	3
Caelo	Hydrophilic ointment DAB	12055801	3
Caelo	Hydrophilic ointment DAB	12055901	10
Fiebig 08.10.12 ek: 10,...	Hydrophilic ointment DAB	12055901	1
Caelo	Hydrophilic ointment DAB	12056001	1
Caesar & Loretz GmbH, 4...	Hydrophilic ointment DAB	12056002	1
Caelo	Hydrophilic ointment DAB	12056002	4
Caelo	Hydrophilic ointment DAB	12086702	3
Caelo	Hydrophilic ointment DAB	12204802	8

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Supplier	Substance	Batch	Spectra
Noweda	Hydrophilic ointment DAB	12204802	2
Caelo	Hydrophilic ointment DAB	12204803	1
Caelo	Hydrophilic ointment DAB	12204901	2
Caelo	Hydrophilic ointment DAB	12205001	6
Caelo	Hydrophilic ointment DAB	12205101	4
Großhandel	Hydrophilic ointment DAB	12205101	1
Caelo	Hydrophilic ointment DAB	12205201	6
Gehe	Hydrophilic ointment DAB	12205201	1
Noweda	Hydrophilic ointment DAB	12205201	1
Caelo	Hydrophilic ointment DAB	12311102	4
Phönix	Hydrophilic ointment DAB	12311301	1
Alliance Healthcare	Hydrophilic ointment DAB	12311102	1
Caelo	Hydrophilic ointment DAB	12311301	6
Caelo	Hydrophilic ointment DAB	12311401	12
Krieger	Hydrophilic ointment DAB	12311401	1
Caelo	Hydrophilic ointment DAB	12311501	14
Doroderm GmbH/ Noweda	Hydrophilic ointment DAB	12311501	1
Caesar&lorenz,Phoenix	Hydrophilic ointment DAB	12311501	1
Caelo	Hydrophilic ointment DAB	12311502	2
Noweda	Hydrophilic ointment DAB	12311502	1
Caelo	Hydrophilic ointment DAB	12311701	7
Caelo	Hydrophilic ointment DAB	12311801	3
Fagron	Hydrophilic ointment DAB	12A12-T03	1
Fagron	Hydrophilic ointment DAB	12C09-T01	2
Noweda	Hydrophilic ointment DAB	12311801	1
Phönix Gotha	Hydrophilic ointment DAB	12G18-T10	1
Fagron	Hydrophilic ointment DAB	12J31-T04	4
Caelo	Hydrophilic ointment DAB	13014001	4
Caelo	Hydrophilic ointment DAB	13013901	2
Gehe 07.05.2013	Hydrophilic ointment DAB	13014002	1
Caelo	Hydrophilic ointment DAB	13014002	9
Caelo	Hydrophilic ointment DAB	13014003	5
Caesar & Loretz GmbH	Hydrophilic ointment DAB	13014002	1
Caelo	Hydrophilic ointment DAB	13014101	6
gehe 11.06.2013	Hydrophilic ointment DAB	13014101	1
Caelo	Hydrophilic ointment DAB	13117102	8
Euro OTC	Hydrophilic ointment DAB	13117102	1
Sanacorp	Hydrophilic ointment DAB	13117102	3
Caelo	Hydrophilic ointment DAB	13117103	4
Caelo	Hydrophilic ointment DAB	13117201	2
Caelo	Hydrophilic ointment DAB	13117301	20
Gehe	Hydrophilic ointment DAB	13117301	2
Anzag 02.10.13	Hydrophilic ointment DAB	13117301	1
Caelo	Hydrophilic ointment DAB	13117401	6
Caesar & Loretz GmbH, 4...	Hydrophilic ointment DAB	13117501	1
Großhandel	Hydrophilic ointment DAB	13117501	1
Caelo	Hydrophilic ointment DAB	13117601	5
Alliance Healthcare	Hydrophilic ointment DAB	13117501	1
Caelo	Hydrophilic ointment DAB	13245302	6
Caelo	Hydrophilic ointment DAB	13245303	1
Caesar&Loretz GmbH/Anzag	Hydrophilic ointment DAB	13245401	1
Caesar&lorenz,Phoenix	Hydrophilic ointment DAB	13245401	1
Caesar & Loretz GmbH	Hydrophilic ointment DAB	13245401	1
Caelo	Hydrophilic ointment DAB	13245801	4
Caelo	Hydrophilic ointment DAB	13246002	4
Fagron	Hydrophilic ointment DAB	13B04-T18-001057	2
Caelo	Hydrophilic ointment DAB	13B04-T18-001061	2
Fagron	Hydrophilic ointment DAB	13E10-T06-003563	1
Fagron	Hydrophilic ointment DAB	13E10-T06-003561	1
Fagron	Hydrophilic ointment DAB	13H13-T04-006144	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydrophilic ointment DAB	15056002	1
Caelo	Hydrophilic ointment DAB	20221110-1	1
Caelo	Hydrophilic ointment DAB	2109212539	1
Caelo	Hydrophilic ointment DAB	25051307	1
Caelo	Hydrophilic ointment DAB	24011315	1
Caelo	Hydrophilic ointment DAB	27121301	1
Bombastus	Hydrophilic ointment DAB	276671	2
Bombastus	Hydrophilic ointment DAB	279002	3
Gehe	Hydrophilic ointment DAB	276671	2
Bombastus	Hydrophilic ointment DAB	279001	2
Bombastus	Hydrophilic ointment DAB	281349	1
Bombastus	Hydrophilic ointment DAB	281350	1
Caelo	Hydrophilic ointment DAB	281351	1
Caelo	Hydrophilic ointment DAB	3613Q2539	1
Caelo	Hydrophilic ointment DAB	4912E-02539	1
Caelo	Hydrophilic ointment DAB	5099200	1
Phönix	Hydrophilic ointment DAB	5321400	1
DAB 2008 Henry Lamotte ...	Hydrophilic ointment DAB	5243000	1
Henry Lamotte/Anzag	Hydrophilic ointment DAB	5321400	1
Lamotte / AHC	Hydrophilic ointment DAB	5448000	1
Lamotte	Hydrophilic ointment DAB	5321400	1
Caelo	Hydrophilic ointment DAB	5448000	1
Lamotte	Hydrophilic ointment DAB	518400	1
Lamotte/Alliance	Hydrophilic ointment DAB	5517900	1
Caelo	Hydrophilic ointment DAB	80127028	1
Bombastus	Hydrophilic ointment DAB	6861252	1
Caelo	Hydrophilic ointment DAB	U-020413-1	1
Phoenix*lamotte	Hydrophilic ointment DAB	5517900	1
Fagron	Hydrophilic ointment DAB		1
Sanacorp	Hydrophilic ointment DAB	AKD32	1
Caelo	Emulsifying hydrophobic base...		1
Fagron	Emulsifying hydrophobic base...	10L14-T54-003418	1
Caelo	Hydrophobic base gel DAC	64/2014	1
Fagron	Hydrophobic base gel DAC	10L14-T54	1
Gehe Kassel	Hydrophobic base gel DAC	271904	1
Bombastus	Hydrophobic base gel DAC	10071402	1
Fagron	Hydrophobic base gel DAC	10L14-T54-006109	2
Caelo	Hydrophobic base gel DAC	10L14-T54-009128	1
Fagron	Hydrophobic base gel DAC	10L14-T54-009128	1
Gehe 23.05.2014	Hydrophobic base gel DAC	14044601	1
Phoenix	Emulsifying hydrophobic base...	14087502	1
Caelo	Hydrophobic base gel DAC	14304603	3
Caelo	Hydrophobic base gel DAC	14304624	1
Caelo	Emulsifying hydrophobic base...	15064001	2
Caelo	Emulsifying hydrophobic base...	15064201	1
Geilenkirchen	Hydrophobic base gel DAC	15064201	1
Caelo	Hydrophobic base gel DAC	15149604	4
Noweda	Hydrophobic base gel DAC	15149604	1
Caelo	Emulsifying hydrophobic base...	15205101	1
Caelo	Hydrophobic base gel DAC	15240802	1
Caelo	Emulsifying hydrophobic base...	15331102	1
Caelo	Hydrophobic base gel DAC	15436102	2
Euro OTC	Hydrophobic base gel DAC	15436102	1
Caelo	Emulsifying hydrophobic base...	15964101	1
Fagron	Hydrophobic base gel DAC	15L10-T04-028696	1
Caelo	Hydrophobic base gel DAC	16054201	2
Fagron	Hydrophobic base gel DAC	16H24-T02-034643	1
Bombastus	Hydrophobic base gel DAC	24031504	1
Bombastus	Hydrophobic base gel DAC	283998	1
Phoenix 02.05.2014	Emulsifying hydrophobic base...	282094	1

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Supplier	Substance	Batch	Spectra
GEHE Kassel	Hydrophobic base gel DAC	289214	1
Bombastus	Hydrophobic base gel DAC	292717	1
Bombastus	Hydrophobic base gel DAC	297433	1
Bombastus	Hydrophobic base gel DAC	300896	1
Caelo	Hydrophobic base gel DAC	12229003	2
Bombastus	Hydrophobic base gel DAC	271904	2
Bombastus	Emulsifying hydrophobic base...	262696	1
Bombastus	Emulsifying hydrophobic base...	271106	2
Bombastus	Emulsifying hydrophobic base...	255106	1
Anzag 05.11.12	Emulsifying hydrophobic base...	271106	1
Fagron	Emulsifying hydrophobic base...	10L14-T54-111713	1
Caelo	Emulsifying hydrophobic base...	11105002	1
Caelo	Emulsifying hydrophobic base...	11016804	1
Bombastus	Emulsifying hydrophobic base...	11071308	1
Bombastus	Emulsifying hydrophobic base...	11041301	1
Fagron	Emulsifying hydrophobic base...	1108-T01	1
Caelo	Emulsifying hydrophobic base...	11209302	1
Fagron	Emulsifying hydrophobic base...	11G25-T01	1
Caelo	Emulsifying hydrophobic base...	11301605	1
Fagron	Emulsifying hydrophobic base...	11I08-T01	2
Caelo	Emulsifying hydrophobic base...	12078001	2
Caelo	Emulsifying hydrophobic base...	12160201	4
Noweda	Emulsifying hydrophobic base...	12160201	1
phoenix	Emulsifying hydrophobic base...	12182301	1
Caelo	Emulsifying hydrophobic base...	12182303	3
Caelo	Emulsifying hydrophobic base...	12229001	4
Caelo	Emulsifying hydrophobic base...	12303402	5
anzag,04.12.12	Emulsifying hydrophobic base...	12229006	1
phönix, 21.01.2013	Emulsifying hydrophobic base...	12303402	1
Gehe	Emulsifying hydrophobic base...	13066802	3
Gehe	Hydrophobic base gel DAC	12F29-T01	1
Fagron	Emulsifying hydrophobic base...	12F29-T01	1
Gehe	Emulsifying hydrophobic base...	13177601	1
Caelo	Emulsifying hydrophobic base...	13177602	1
Caelo	Hydrophobic base gel DAC	13165205	1
Sanacorp	Emulsifying hydrophobic base...	13177601	1
Caelo	Hydrophobic base gel DAC	13295701	1
Caelo	Emulsifying hydrophobic base...	13341701	2
Caelo	Emulsifying hydrophobic base...	13341703	3
Noweda	Emulsifying hydrophobic base...	13361004	1
Bombastus	Emulsifying hydrophobic base...	22111307	1
Bombastus	Emulsifying hydrophobic base...	277443	1
Caelo	Emulsifying hydrophobic base...	28051301	1
Apomix	Eye ointment, emulsifying DAC	3A180213	1
Caelo	Paraffin, white	13268422	4
Euro OTC	Wool alcohol ointment DAB	1211017-01	3
Caelo	Wool alcohol ointment DAB	12340101	6
Caelo	Wool alcohol ointment DAB	15035502	9
Caelo	Wool alcohol ointment DAB	15225401	2
Caelo	Wool alcohol ointment DAB	15228201	5
Beiersdorf AG	Wool alcohol ointment DAB	15362002	1
Caelo	Wool alcohol ointment DAB	16198502	2
Bombastus	Wool alcohol ointment DAB	296437	2
Bombastus	Wool alcohol ointment DAB	301202	2
Bombastus	Wool alcohol ointment DAB	295218	2
Beiersdorf AG	Wool alcohol ointment DAB	50444710	1
Beiersdorf/Phönix	Wool alcohol ointment DAB	60429110	1
Anzag/Beiersdorf	Wool alcohol ointment DAB	50815310	1
Beiersdorf/Phoenix	Wool alcohol ointment DAB	61149910	1
Beiersdorf/Phoenix	Wool alcohol ointment DAB	63052310	1

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Supplier	Substance	Batch	Spectra
Bombastus	Wool alcohol ointment DAB	265368	1
Caelo	Wool alcohol ointment DAB	11335002	6
Bombastus	Wool alcohol ointment DAB	270643	3
Holdermann/Beiersdorf	Wool alcohol ointment DAB	22532710	1
Beiersdorf/N/22.03.2013...	Wool alcohol ointment DAB	24635410	1
Apomix/ Phönix	Eye ointment, emulsifying DAC	3C200114	2
Apomix/Noweda	Eye ointment, emulsifying DAC	15C030815	1
Apomix/Kehr	Eye ointment, emulsifying DAC	15B030815	1
Euro OTC	Eye ointment, emulsifying DAC	18A021115	1
Apomix/Sanacorp 13.05.2...	Eye ointment, emulsifying DAC	3270115	1
PKH/ Noweda	Eye ointment, emulsifying DAC	12E010814	1
AMH Niemann/E	Eye ointment, emulsifying DAC	1C080114	1
PKH Halle/ Phoenix	Eye ointment, emulsifying DAC	3A180213	1
Phönix Gotha	Eye ointment, emulsifying DAC	5B220413	1
apomix/Phönix	Eye ointment, emulsifying DAC	11A170713	1
PKH Gmbh/Phönix	Eye ointment, emulsifying DAC	7B210513	1
PKH Halle/ Phoenix	Eye ointment, emulsifying DAC	11D170713	1
Phönix Gotha	Eye ointment, emulsifying DAC	16B061212	1
PKH GmbH/ Phönix	Eye ointment, emulsifying DAC	12C300813	1
Apomix / Phönix	Eye ointment, emulsifying DAC	17C061212	2
Apomix /	Eye ointment, emulsifying DAC	17B111113	1
Caelo	Paraffin		2
Bombastus	Paraffin	260652	1
Bombastus	Paraffin	263350	1
Bombastus	Paraffin	272590	1
Phoenix, 04.08.2012	Paraffin	269213	2
Noweda	Paraffin	122875	1
Fagron	Paraffin	941435	1
Bombastus	Paraffin	266032	1
Henry Lamotte	Paraffin	122587	1
Gehe	Paraffin	122875	1
Henry Lamotte GmbH, Mer...	Paraffin	122875	1
Henry Lamotte	Paraffin	122875	2
Lamotte	Paraffin	123075	1
Henry Lamotte	Paraffin	123075	1
Noweda / Henry Lamotte	Paraffin	123075	2
Henry Lamotte Oils GmbH	Paraffin	122875	1
H.Lamotte/Noweda	Paraffin	123075	1
Henry Lamotte oils GmbH	Paraffin	123075	2
Henry Lamotte Oils GmbH	Paraffin	123075	1
Phönix	Paraffin	123075	1
Henry Lamotte	Paraffin	123393	1
Phönix	Paraffin	123393	2
Henry Lamotte Oels GmbH	Paraffin	123393	1
Henry Lamotte	Paraffin	123743	10
Henry Lamotte oils GmbH	Paraffin	123743	8
Lamotte	Paraffin	123743	1
Henry Lamotte Oils GmbH...	Paraffin	123743	3
Henry Lamotte / Noweda	Paraffin	123743	4
Henry Lamotte GmbH, Mer...	Paraffin	123743	1
Noweda	Paraffin	123743	1
Oils/ Phönix	Paraffin	123743	2
Henry Lamotte Oils GmbH...	Paraffin	123743	1
Henry Lamotte Oils / No...	Paraffin	123743	2
Lamotte/Anzag	Paraffin	123743	1
Caelo	Paraffin	123743	1
Caelo	Paraffin	214U-02050	1
Caelo	Paraffin	2111202	1
Lamotte / Alliance Heal...	Paraffin	125544	1
Eigenherstellung	Paraffin	60614HJK01	1

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Supplier	Substance	Batch	Spectra
Bombastus	Paraffin	6861849	2
Caelo	Paraffin	4091515	1
Caelo	Paraffin	9320905	1
Caelo	Paraffin	715I-02050	1
Fagron	Paraffin	1004C014	1
Eigenherstellung	Paraffin	100615HJK01	1
Caelo	Paraffin	10071202	1
Caelo	Paraffin	10071403	1
Caelo	Paraffin	10162002	1
Caelo	Paraffin	10364703	1
Caelo	Paraffin	11071302	1
Caelo	Paraffin	11009510	1
Euro OTC	Paraffin	1106009-01	1
Fagron	Paraffin	110816-2	1
Caelo	Paraffin	11092703	1
Hersteller: EuRho	Paraffin	1110014-01	1
Euro OTC	Paraffin	1110014-01	2
Europharm/Otto	Paraffin	1110014-01	1
Caelo	Paraffin	1114U02050	1
Caelo	Paraffin	11207702	3
Eigenherstellung	Paraffin	11214HAS01	1
Caelo	Paraffin	11263606	4
Caelo	Paraffin	11354102	7
Gehe	Paraffin	11354102	1
Noweda	Paraffin	11354102	1
Caelo	Paraffin	1135412	1
Caelo	Paraffin	113544102	1
Fagron	Paraffin	11co8-no7	1
Fagron	Paraffin	11f30-n03	1
Caelo	Paraffin	11H04-N02	1
Euro OTC	Paraffin	1203042-01	3
Kehr	Paraffin	11H04-N02	1
Fagron	Paraffin	11L19-N01	1
Phoenix	Paraffin	12042202	1
Caelo	Paraffin	12042202	19
EuRho	Paraffin	1203042-01	1
Anzag 02.01.2013	Paraffin	12042202	1
Caelo	Paraffin	12042205	4
Caelo	Paraffin	1205033-01	1
Gehe	Paraffin	1207022-01	2
EuRho	Paraffin	1207022-01	1
Euro OTC	Paraffin	1207022-01	2
Noweda	Paraffin	1208021-01	3
Gehe	Paraffin	1208021-01	1
Euro OTC	Paraffin	1208021-01	3
Caelo	Paraffin	12102101	10
Caelo	Paraffin	12109603	2
Euro OTC	Paraffin	1211026-01	6
Gehe	Paraffin	1211026-01	1
Euro OTC	Paraffin	1211027-01	7
Phönix/Euro	Paraffin	1211027-01	1
Europharm/Otto	Paraffin	1211027-01	1
Euro OTC	Paraffin	121102701	1
Noweda	Paraffin	1211027-01	1
Caelo	Paraffin	12227602	1
Caelo	Paraffin	12227601	2
Caelo	Paraffin	12227609	5
Gehe 16.04.2013	Paraffin	12227609	1
Caelo	Paraffin	12227610	1
Caelo	Paraffin	12227701	11

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Supplier	Substance	Batch	Spectra
Caelo	Paraffin	12324304	1
GEHE	Paraffin	12324307	1
Caelo	Paraffin	12324307	21
Phönix Gotha	Paraffin	12324307	1
Gehe	Paraffin	12324307	1
Caelo	Paraffin	1234307	1
Laborchemie Apolda/Jenn...	Paraffin	12345	1
Caelo	Paraffin	1235465	1
Fagron	Paraffin	123586	3
Anzag	Paraffin	123586	1
Euro OTC	Paraffin	125071	1
Caelo	Paraffin	12H27-N01	2
Euro OTC	Paraffin	125962	1
Fagron	Paraffin	12H27-N01	8
Fagron	Paraffin	12H27-N01	1
Fagron	Paraffin	12J23-N03	4
Caelo	Paraffin	13005805	13
Caelo	Paraffin	13005205	1
Lamotte	Paraffin	13005805	1
Cealo	Paraffin	1300805	1
Caelo	Paraffin	13005806	1
Hedinger/Phönix	Paraffin	1302C008-279571	1
Noweda	Paraffin	1303031-01	1
Euro OTC	Paraffin	1303031-01	8
Euro OTC	Paraffin	130303101	1
Euro OTC	Paraffin	1304010-01	4
Caelo	Paraffin	13050102	20
PHÖNIX 05.06.2013	Paraffin	13050102	1
Euro OTC	Paraffin	1307007-01	10
Eigenherstellung	Paraffin	130712HML01	1
Euro OTC	Paraffin	1309022-01	2
Caelo	Paraffin	1309022-02	2
Euro OTC	Paraffin	130902201	1
Caelo	Paraffin	13103309	15
Spinnrad	Paraffin	13103308	1
Gehe	Paraffin	13103309	1
Euro OTC	Paraffin	1311024-01	9
EuRho / Noweda	Paraffin	131102401	1
Caelo	Paraffin	1311024-01	2
Euro OTC	Paraffin	131102401	2
Caelo	Paraffin	13131704	1
Phönix	Paraffin	13131705	1
Caelo	Paraffin	13131705	15
Caelo	Paraffin	1313705	1
Henry Lamotte Oils GmbH...	Paraffin	13148606	1
Caelo	Paraffin	1322902	1
Caelo	Paraffin	13232901	14
Caelo	Paraffin	13232902	11
Caelo	Paraffin	13232903	6
Caelo	Paraffin	13248006	1
Caelo	Paraffin	13248007	8
Euro OTC	Paraffin	133888	1
Caelo	Paraffin	13390601	6
Caelo	Paraffin	13390602	14
Cealo	Paraffin	13390602	1
Gehe	Paraffin	13390602	1
Sanacorp	Paraffin	13390602	1
Caelo	Paraffin	13390604	1
Devesa/Kehr	Paraffin	13390602	1
Caelo	Paraffin	13390606	1

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Supplier	Substance	Batch	Spectra
Fagron	Paraffin	13A3010	2
Fagron	Paraffin	13A30-N11	14
Fargon	Paraffin	13A30-N11	1
Phönix	Paraffin	13A30-N11	2
Phoenix	Paraffin	13A30-N11	1
Fagron	Paraffin	13a30-n11	1
Großhandel	Paraffin	13C19-N09	1
Fagron	Paraffin	13C19-N09	3
Pönix 10.06.2013	Paraffin	13C19-N09	1
Fagron	Paraffin	13E28-N02	12
Sanacorp	Paraffin	13E28-N02	1
Fagron	Paraffin	13G24-N12	4
Fagron	Paraffin	13G24N12	1
Caelo	Paraffin	13G24-N12	2
Gehe	Paraffin	13G24-N12	1
Fagron	Paraffin	13L17-B01-289491	4
Caelo	Paraffin	13L17-B01	1
Fagron	Paraffin	13L17-B01	1
Fagron	Paraffin	13H02-B02	1
Fagron	Paraffin	13L17-B01-289492	3
Fiebig	Paraffin	13L17-B01-289492	1
Fagron	Paraffin	13L17-b01-289492	1
Fagron	Paraffin	13L17-B01-289492	1
Fagron	Paraffin	13L17-B01-289493	4
Caelo	Paraffin	14011303	1
Euro OTC	Paraffin	1404009-01	7
Caelo	Paraffin	14011514	1
Caelo	Paraffin	1404009-01	1
Euro OTC	Paraffin	140400901	1
Noweda	Paraffin	1404009-09	1
Euro OTC	Paraffin	1404010-01	1
Euro OTC	Paraffin	140401001	2
Fagron	Paraffin	1404010-01	1
Caelo	Paraffin	14044504	2
Caelo	Paraffin	14044507	4
Caelo	Paraffin	14059701	4
Phoenix 10.10.14	Paraffin	14059701	1
Phönix	Paraffin	14059701	1
Caelo	Paraffin	14059703	2
Caelo	Paraffin	14059705	1
Caelo	Paraffin	14059708	4
Caesar&loretz,Anzag	Paraffin	14059708	1
Euro OTC	Paraffin	14059708	1
Euro OTC	Paraffin	1407042-01	6
Caelo	Paraffin	1407042-01	1
Euro OTC	Paraffin	1412010-01	6
Euro OTC	Paraffin	140900701	1
Euro/ Sanacorp	Paraffin	1409007-01	1
Caelo	Paraffin	14134601	1
Caelo	Paraffin	14141408	2
Caelo	Paraffin	14163804	5
Caelo	Paraffin	14163807	10
Bombastus	Paraffin	14187601	1
Caelo	Paraffin	14202507	6
Caelo	Paraffin	14202509	10
Caelo	Paraffin	14305904	3
Caelo	Paraffin	14305905	6
Caelo	Paraffin	14357203	8
Noweda 19.05.2015	Paraffin	14357203	1
Caelo	Paraffin	14357204	6

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Supplier	Substance	Batch	Spectra
Caelo	Paraffin	14357205	2
Fagron	Paraffin	14357205	1
Caelo	Paraffin	1437205	1
Fagron	Paraffin	14D24-B05	6
Caelo	Paraffin	14D24-B05-295022	1
Fagron	Paraffin	14D24-B05-295014	3
Fagron	Paraffin	14D24-B05-295022	2
Caelo	Paraffin	14D24B05-295022	1
Fagron	Paraffin	14d24-b05-295023	1
Fagron	Paraffin	14D24-B05-295023	3
Hansen & Rosenthal KG/N...	Paraffin	14D24-B05-295023	1
Fagron	Paraffin	14D24-B05-295023	1
Devesa/ Phönix	Paraffin	14D24-B05-295022	1
Euro Pharma	Paraffin	150101601	1
Euro OTC	Paraffin	1501016-01	3
Euro OTC	Paraffin	150101601	1
Eigenherstellung	Paraffin	150114HML01	1
Euro OTC	Paraffin	1503046-01	5
Eu Rho/ Gehe	Paraffin	1503046-01	1
Caelo	Paraffin	1503046-01	1
Eigenherstellung	Paraffin	150413HML01	1
Euro OTC	Paraffin	1506005-01	3
EuRho/Phönix	Paraffin	1506005-01	1
Caelo	Paraffin	150600501	1
Bombastus	Paraffin	150600501	1
Euro OTC	Paraffin	1509011-01	1
Caelo	Paraffin	151060104	1
Caelo	Paraffin	15106101	3
Caelo	Paraffin	15106102	1
Caelo	Paraffin	15106104	4
Caelo	Paraffin	15106107	4
Caelo	Paraffin	15106109	6
Euro OTC	Paraffin	1511029-01	2
Euro OTC	Paraffin	1511030-01	7
Caelo	Paraffin	15234502	3
Caesar&Loretz GmbH	Paraffin	15234502	1
Caelo	Paraffin	15234506	1
Caelo	Paraffin	15293201	4
Caelo	Paraffin	15293202	5
Phoenix	Paraffin	15293202	2
Caelo	Paraffin	15293203	7
Caelo	Paraffin	15293204	4
Caelo	Paraffin	15293205	6
Caelo	Paraffin	15299201	1
Caelo	Paraffin	15336703	6
Noweda	Paraffin	15336703	1
Caelo	Paraffin	15336704	1
Calo	Paraffin	15429603	1
Caelo	Paraffin	15429603	1
Fagron	Paraffin	15B16-B03-304611	6
Caelo	Paraffin	16/080/P	1
Euro OTC	Paraffin	1602026-01	4
Caelo	Paraffin	1602026-01	1
Caelo	Paraffin	1601312050	1
Euro OTC	Paraffin	1604009-01	3
Bombastus	Paraffin	1604009-01	1
Euro OTC	Paraffin	1604045-01	2
Caelo	Paraffin	1604045-01	1
Bombastus	Paraffin	1606032-01	1
Euro OTC	Paraffin	1606032-01	1

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Supplier	Substance	Batch	Spectra
Caelo	Paraffin	16061203	1
Euro OTC	Paraffin	1607039-01	1
Caelo	Paraffin	16082904	6
Euro OTC	Paraffin	160703901	1
AHD	Paraffin	16082904	1
Phoenix	Paraffin	16082906	1
Caelo	Paraffin	16082908	2
Caelo	Paraffin	16082907	1
Phoenix	Paraffin	16082907	1
Caelo	Paraffin	16082905	1
Caelo	Paraffin	16149802	5
Ebert KKH 30.09.16	Paraffin	16149802	1
Hansen & Rosenthal/Noweda	Paraffin	16A27-B01	1
Fagron	Paraffin	16A27-B01-323777	1
Caelo	Paraffin	1811Q-02050	1
Fagron	Paraffin	16E30-B05-324041	1
Caelo	Paraffin	19021302	1
Caelo	Paraffin	1913Q-02050	1
Henry Lamotte Olis	Paraffin	2x5367601	1
fargon	Paraffin	196310	1
Caelo	Paraffin	2103312050	1
Euro OTC	Paraffin	22101402	1
Caelo	Paraffin	20210312-4	1
Caelo	Paraffin	221108111F30-N0	1
Eigenherstellung	Paraffin	210714H01	1
Eigenherstellung	Paraffin	240715HML01	1
Caelo	Paraffin	2213A-02050	1
Caelo	Paraffin	25092015	1
Eigenherstellung	Paraffin	260115ML01	1
Eigenherstellung	Paraffin	261113HML01	1
Euro OTC	Paraffin	261113PML01	1
Caelo	Paraffin	27011405	1
Bombastus	Paraffin	274958	5
Pönix 10.05.2013	Paraffin	274958	1
A.H. 03.06.13 ek: 6,15EUR	Paraffin	274958	1
Bombastus	Paraffin	281540	3
Bombastus	Paraffin	284273	1
Bombastus	Paraffin	288827	2
Bombastus	Paraffin	290824	2
Eigenherstellung	Paraffin	291012HJK01	1
Bombastus	Paraffin	292137	1
Bombastus	Paraffin	293385	1
Bombastus	Paraffin	295576	1
Bombastus	Paraffin	298396	1
Bombastus	Paraffin	300061	1
Caelo	Paraffin	3213Q2050	1
Caelo	Paraffin	3613A-02050	1
fragon	Paraffin		1
Caelo	Paraffin	4112M-02048	1
Fagron	Paraffin	4413M2050	1
Henry Lamotte Oils GmbH	Paraffin	5098101	1
Henry Lamotte/Anzag	Paraffin	5367601	3
Phönix/Henry	Paraffin	5367601	7
Henry Lamotte	Paraffin	5367601	10
Henry Lamotte GmbH, Mer...	Paraffin	5367601	2
Phönix/Lamotte	Paraffin	5367601	2
Henry Lamotte/GEHE	Paraffin	5367601	2
Kehr	Paraffin	5367601	1
Alliance Healthcare	Paraffin	5367601	2
Caelo	Paraffin	5367601	2

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Supplier	Substance	Batch	Spectra
Lamotte	Paraffin	5367601	4
Lamotte/GEHE	Paraffin	5367601	1
Henry Lamotte Olis GmbH	Paraffin	5367601	2
Sanacorp	Paraffin	5367601	1
LAMOTTE/NOWEDA	Paraffin	5367601	1
Henry Lamotte Oils/Phönix	Paraffin	5367601	1
H.Lamotte/Noweda	Paraffin	5367601	1
Hedinger	Paraffin	5367601	1
Henry Lamotte	Paraffin	5593601	5
Henry Lamotte Oils GmbH	Paraffin	5367601	1
Henry Lamotte Olis GmbH...	Paraffin	5593601	2
Caelo	Paraffin	5593601	1
lamotte noweda,	Paraffin	5593601	1
Lamotte/Gehe	Paraffin	5593601	1
Noweda / Henry Lamotte ...	Paraffin	5593601	1
Sanacorp	Paraffin	5593601	2
Henry Lamotte oils GmbH...	Paraffin	5593601	5
Lamotte / Noweda	Paraffin	5593601	1
Noweda/Lamotte	Paraffin	5593601	1
Alliance health	Paraffin	5593601	1
Henry Lamotte/Sana	Paraffin	5593601	2
Lamotte / Alliance Heal...	Paraffin	5593601	1
Caelo	Paraffin	57/AD1	1
Caelo	Paraffin	58/AKD55	1
Caelo	Paraffin	59/AKD2	1
Sanacorp	Paraffin	59/AKD4	1
Henry Lamotte/Phönix	Paraffin	7316019	1
Caelo	Paraffin	83054508	1
Henry Lamotte GmbH, Mer...	Paraffin	79460	1
Fagron	Paraffin	959561	3
Phoenix	Paraffin	959561	1
Euro OTC	Paraffin	Ch1211026-01	1
Eigenherstellung	Paraffin		1
Euro OTC	Paraffin	1102009-01	1
Herbasinica	Paraffin	11354102	1
EUro/AHD	Paraffin	1211027-01	1
Sanacorp	Paraffin	1211027-01	1
Sanacorp	Paraffin	1304010-01	1
Gutenberg-Apotheke	Paraffin	13248007	1
Fagron	Paraffin	13E28-N02	1
Caeo	Paraffin	14305905	1
Euro OTC	Paraffin	1506021-01	1
Euro	Paraffin	1511030-01	1
HansenRosenthalKG/Hansen	Hydrophobic base gel DAC	1078667	1
ICHTHYOL-GESELLSCHAFT C...	Fatty ointment anhydrous, wa...	13A089	1
Ichthyol	Fatty ointment anhydrous, wa...	13A091	1
Caelo	Fatty ointment anhydrous, wa...	13A113	1
Ichthyol-Gesellschaft	Fatty ointment anhydrous, wa...	13A172	1
Ichthyol Gesellschaft	Fatty ointment anhydrous, wa...	13A171	1
Ichthyol Gesellschaft/AHD	Fatty ointment anhydrous, wa...	13A180	1
Fagron	Wool alcohol ointment DAB	13D09-T04-007315	1
Ichthyol/gehe	Fatty ointment anhydrous, wa...	14A005	1
Caelo	Fatty ointment anhydrous, wa...	14A095	1
Ichthyol/gehe	Fatty ointment anhydrous, wa...	14A099	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	15A020	2
AHD	Fatty ointment anhydrous, wa...	15A021	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	15A023	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	15A062	1
A.H.D.	Fatty ointment anhydrous, wa...	15A060	1
Ichthyol/ AHD	Fatty ointment anhydrous, wa...	15A091	1

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Supplier	Substance	Batch	Spectra
Ichtyol/Phönix	Fatty ointment anhydrous, wa...	15A029	1
ICHTHYOL-GESELLSCHAFT	Fatty ointment anhydrous, wa...	15A042	1
ICHTHYOL-GESELLSCHAFT	Fatty ointment anhydrous, wa...	15A091	1
ICHTHYOL-GESELLSCHAFT C...	Fatty ointment anhydrous, wa...	15A123	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	15A124	1
Caelo	Fatty ointment anhydrous, wa...	15A123	1
ICHTHYOL-GESELLSCHAFT C...	Fatty ointment anhydrous, wa...	15A124	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	15A162	1
ICHTHYOL-GESELLSCHAFT	Fatty ointment anhydrous, wa...	15A156	1
ICHTHYOL-GESELLSCHAFT	Fatty ointment anhydrous, wa...	15A191	1
Ichtyol/Gehe	Fatty ointment anhydrous, wa...	15A78	1
Caelo	Hydrophilic ointment DAB	16009401	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	16A023	1
Galderma/Phönix	Fatty ointment anhydrous, wa...	16A077	1
ICHTHYOL-GESELLSCHAFT C...	Fatty ointment anhydrous, wa...	16A083	1
ICHTHYOL-GESELLSCHAFT/P...	Fatty ointment anhydrous, wa...	16A140	1
ICHTHYOL-GESELLSCHAFT/P...	Fatty ointment anhydrous, wa...	16A173	1
Apomix	Eye ointment, emulsifying DAC	17A111113	1
Apomix	Eye ointment, emulsifying DAC	18B021214	1
Fagron	Wool alcohol ointment DAB	23033310	1
Bombastus	Wool alcohol ointment DAB	279928	3
Bombastus	Wool alcohol ointment DAB	283619	3
Bombastus	Wool alcohol ointment SR wit...	285952	2
Bombastus	Hydrophilic ointment DAB	286543	1
Bombastus	Wool alcohol ointment DAB	287619	2
Bombastus	Wool alcohol ointment DAB	290735	1
Bombastus	Wool alcohol ointment SR wit...	291177	2
Bombastus	Wool alcohol ointment DAB	291795	4
Beiersdorf	Wool alcohol ointment DAB	42541910	1
Beiersdorf/Gehe	Wool alcohol ointment DAB	40726610	1
Lamotte/Anzag	Hydrophilic ointment DAB	5112A-02539	1
Lamotte	Hydrophilic ointment DAB	5651600	2
Henry Lamotte Oils	Hydrophilic ointment DAB	5860400	2
Beiersdorf	Wool alcohol ointment DAB	11235310	1
Caelo	Wool alcohol ointment DAB	13242603	4
Beiersdorf/AHD	Wool alcohol ointment DAB	22412510	1
Beiersdorf	Wool alcohol ointment DAB	24655410	1
Gehe	Wool alcohol ointment SR wit...	276135	1
Bombastus	Wool alcohol ointment SR wit...	277022	2
Sanacorp	Wool alcohol ointment DAB	277190	2
Bombastus	Wool alcohol ointment DAB	279105	3
Sanacorp	Wool alcohol ointment DAB	279927	1
Bombastus	Wool alcohol ointment SR wit...	283176	3
Bombastus	Wool alcohol ointment SR wit...	280059	1
Beiersdorf, Phönix	Wool alcohol ointment DAB	30721310	1
Beiersdorf, Phönix	Wool alcohol ointment DAB	31121710	1
Beiersdorf	Wool alcohol ointment DAB	31121710	1
Beiersdorf	Wool alcohol ointment DAB	31241810	2
Ichthyol/Anzag	Fatty ointment anhydrous, wa...	12A055	1
Sanova	Fatty ointment anhydrous, wa...	11A040	1
Ichthyol/N/14.02.13	Fatty ointment anhydrous, wa...	12A131	1
ichthyol	Fatty ointment anhydrous, wa...	12A115	1
Gehe	Fatty ointment anhydrous, wa...	11A161	1
Ichtyol-Gesellschaft	Fatty ointment anhydrous, wa...	12A184	1
Caelo	Fatty ointment anhydrous, wa...	13A004	1
Ichthyol Jenne	Fatty ointment anhydrous, wa...	12A211	1
Ichthyol/Phönix	Fatty ointment anhydrous, wa...	13A010	1
Sanacorp	Fatty ointment anhydrous, wa...	13A042	1
ichthyol/N/PZN:01062983	Fatty ointment anhydrous, wa...	13A050	1
Ichthyl Phönix	Fatty ointment anhydrous, wa...	13A053	1

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Supplier	Substance	Batch	Spectra
Ichthyol	Fatty ointment anhydrous, wa...	13A109	1
Ichthyol/gehe	Fatty ointment anhydrous, wa...	13A114	1
ichthyol/AHD	Fatty ointment anhydrous, wa...	13A109	1
Bombastus	Hydrophilic ointment DAB	269534	2
Anzag	Hydrophilic ointment DAB	271047	1
Bombastus	Hydrophilic ointment DAB	274002	1
Bombastus	Hydrophilic ointment DAB	274003	1
Caelo	Hydrophilic ointment DAB	13171102	1
Bombastus	Hydrophilic ointment DAB	276670	1
Bombastus	Hydrophilic ointment DAB	279000	2
Apomix	Eye ointment, emulsifying DAC	15A241013	1
Apomix	Eye ointment, emulsifying DAC	5B220413	1
Bombastus	Paraffin, white	258194	1
Gehe	Paraffin, white	261731	1
Noweda	Paraffin, white	263762	1
Bombastus	Paraffin, white	263759	1
Noweda	Paraffin, white	255510	1
Bombastus	Paraffin, white	265508	1
Bombastus	Paraffin, white	265814	1
Bombastus	Paraffin, white	267010	2
Bombastus	Paraffin, white	268016	1
Bombastus	Paraffin, white	268099	2
Bombastus	Paraffin, white	268390	1
Gehe	Paraffin, white	268099	1
Bombastus	Paraffin, white	269731	2
Bombastus	Paraffin, white	269732	3
Gehe	Paraffin, white	268391	1
Bombastus	Paraffin, white	269733	3
Bombastus	Paraffin, white	269734	5
Bombastus	Paraffin, white	270163	1
Noweda	Paraffin, white	270163	3
Bombastus	Paraffin, white	270165	2
Bombastus	Paraffin, white	270490	1
Bombastus	Paraffin, white	270489	2
Phoenix	Paraffin, white	270491	1
Bombastus	Paraffin, white	270491	1
Anzag 08.10.12	Paraffin, white	270491	1
Bombastus	Paraffin, white	270633	1
Phönix Gotha	Paraffin, white	270633	1
Bombastus	Paraffin, white	270634	1
Phönix Gotha	Paraffin, white	270634	1
Bombastus	Paraffin, white	270635	2
Bombastus	Paraffin, white	270834	3
Bombastus	Paraffin, white	270976	4
Bombastus	Paraffin, white	270835	1
Bombastus	Paraffin, white	270978	3
Bombastus	Paraffin, white	270977	1
Bombastus	Paraffin, white	270979	4
Bombastus	Paraffin, white	270982	3
Bombastus	Paraffin, white	271213	4
Bombastus	Paraffin, white	271260	1
Bombastus	Paraffin, white	271261	2
Noweda	Paraffin, white	271261	1
Gehe	Paraffin, white	271435	1
Bombastus	Paraffin, white	271435	2
Anzag	Paraffin, white	271435	1
Bombastus	Paraffin, white	271437	5
Caelo	Paraffin, white	1021302	1
Caelo	Paraffin, white	1061301	1
Caelo	Paraffin, white	1081409	1

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Supplier	Substance	Batch	Spectra
Caelo	Paraffin, white	2061201	1
Caelo	Paraffin, white	213E-02549	1
Caelo	Paraffin, white	3071202	1
Caelo	Paraffin, white	3091209	1
Caelo	Paraffin, white	402312550	1
Caelo	Paraffin, white	4031406	1
Hedinger/Noweda	Paraffin, white	4-219072	1
Caelo	Paraffin, white	5061412	1
Caelo	Paraffin, white	6061302	1
Caelo	Paraffin, white	5041303	1
Caelo	Paraffin, white	613Q-02549	1
Bombastus	Paraffin, white	6861393	1
Caelo	Paraffin, white	713I-02549	1
Caelo	Paraffin, white	8021401	1
Caelo	Paraffin, white	8031302	1
Caelo	Paraffin, white	8051303	1
Caelo	Paraffin, white	8101302	1
Caelo	Paraffin, white	813E-02549	1
Caelo	Paraffin, white	100/AKD8	1
Caelo	Paraffin, white	9274706	1
Caelo	Paraffin, white	10051402	1
Bombastus	Paraffin, white	1001312549	1
Caelo	Paraffin, white	10071304	1
Caelo	Paraffin, white	10091301	1
Caelo	Paraffin, white	10071305	1
Caelo	Paraffin, white	10094704	1
Caelo	Paraffin, white	10155402	1
Sanacorp	Paraffin, white	102/AKD1	1
Caelo	Paraffin, white	10220214	1
Caelo	Paraffin, white	10271001	1
Fagron	Paraffin, white	10H12-T01	1
Caelo	Paraffin, white	11011309	1
Caelo	Paraffin, white	11031403	1
Caelo	Paraffin, white	1101559	1
Caelo	Paraffin, white	11040603	1
Caelo	Paraffin, white	11041302	1
Anzag	Paraffin, white	1105029-01	1
Caelo	Paraffin, white	11060209	3
Caelo	Paraffin, white	11060210	3
Caelo	Paraffin, white	11060212	2
Caelo	Paraffin, white	11060211	1
Caelo	Paraffin, white	11060213	6
Euro OTC	Paraffin, white	1108046-01	3
Euro OTC	Paraffin, white	1109002-01	2
Hansen&Rosenthal/Phönix	Paraffin, white	1108046-01	1
Caelo	Paraffin, white	11104901	1
Caelo	Paraffin, white	11091402	1
Caelo	Paraffin, white	11104904	2
Caelo	Paraffin, white	11104910	1
Caelo	Paraffin, white	11108710	1
Caelo	Paraffin, white	11108711	1
Caelo	Paraffin, white	11190913	1
Caelo	Paraffin, white	11115501	1
Caelo	Paraffin, white	11265701	1
Caelo	Paraffin, white	11265703	1
Caelo	Paraffin, white	11265708	2
vdl	Paraffin, white	11265710	1
Caelo	Paraffin, white	11301301	5
Caelo	Paraffin, white	11283902	1
Caesar & Loretz GmbH, 4...	Paraffin, white	11301301	1

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Supplier	Substance	Batch	Spectra
Caelo	Paraffin, white	11265711	1
Noweda	Paraffin, white	11301301	1
Gehe	Paraffin, white	11315403	1
Caelo	Paraffin, white	11315402	1
Caelo	Paraffin, white	11315401	2
Caelo	Paraffin, white	11315408	3
Caelo	Paraffin, white	11315412	1
Caelo	Paraffin, white	11315413	2
Caelo	Paraffin, white	11374901	1
Caelo	Paraffin, white	11374903	4
Caelo	Paraffin, white	11374906	5
Noweda	Paraffin, white	11374906	1
Fagron	Paraffin, white	11G11-T02	2
Fagron	Paraffin, white	11K14-T01	7
Fagron	Paraffin, white	12/17-T01	1
Phönix 08.04.2013	Paraffin, white	12/17-T01	1
Fagron	Paraffin, white	12/17-To1	1
Caesar&lorenz,Anzag	Paraffin, white	12003601	2
Caelo	Paraffin, white	12003603	1
Euro OTC	Paraffin, white	1201035-01	1
Caelo	Paraffin, white	12012604	5
Caelo	Paraffin, white	12012605	1
Caelo	Paraffin, white	12012609	8
Caelo	Paraffin, white	12012707	2
Caelo	Paraffin, white	12031202	1
Caelo	Paraffin, white	12032404	3
Gehe	Paraffin, white	12032404	1
Sanacorp	Paraffin, white	12031506	1
Caelo	Paraffin, white	12032412	2
Caelo	Paraffin, white	12032405	1
Erika apotheke	Paraffin, white	12032413	1
Caelo	Paraffin, white	12032413	21
ANZAG	Paraffin, white	12032413	1
Phönix Gotha	Paraffin, white	12032413	1
Phönix	Paraffin, white	12032413	1
Caelo	Paraffin, white	12033809	1
Caelo	Paraffin, white	1203412	1
Caelo	Paraffin, white	1203413	1
Euro OTC	Paraffin, white	1205048-01	3
Gehe	Paraffin, white	1205048-01	1
Caelo	Paraffin, white	12061201	1
Caelo	Paraffin, white	12071804	1
Caelo	Paraffin, white	12071805	3
Caesar & Loretz GmbH, 4...	Paraffin, white	12071805	1
Caelo	Paraffin, white	12078105	1
Caelo	Paraffin, white	12081404	1
Caelo	Paraffin, white	12081601	3
Euro OTC	Paraffin, white	1210006-01	9
Euro OTC	Paraffin, white	1210010-01	1
Euro OTC	Paraffin, white	1210009-01	3
Caelo	Paraffin, white	12111203	1
Großhandel	Paraffin, white	12115101	1
Caelo	Paraffin, white	12111307	1
Caelo	Paraffin, white	12115101	9
Anzag 27.03.13 ek: 3,66EUR	Paraffin, white	12115101	1
Caelo	Paraffin, white	12115102	16
Caelo	Paraffin, white	12115105	1
Noweda	Paraffin, white	12115106	1
Caelo	Paraffin, white	12115106	7
Gehe	Paraffin, white	12115106	1

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Supplier	Substance	Batch	Spectra
Doroderm GmbH/ Noweda	Paraffin, white	12115106	2
GEHE	Paraffin, white	12115106	1
Sanacorp	Paraffin, white	12115107	1
Caelo	Paraffin, white	12115107	9
Fiebig 22.02.13 ek:3,63EUR	Paraffin, white	12115107	1
Phönix	Paraffin, white	12115107	1
Fagron	Paraffin, white	12115107	1
Caelo	Paraffin, white	12115108	5
Caelo	Paraffin, white	12115113	1
Caelo	Paraffin, white	12121201	1
Caelo	Paraffin, white	12121204	1
Caelo	Paraffin, white	12182504	1
Sanacorp	Paraffin, white	1215107	1
Caelo	Paraffin, white	12182505	7
Anzag/	Paraffin, white	12182505	2
Noweda	Paraffin, white	12182505	1
Caelo	Paraffin, white	12190401	4
Sanacorp	Paraffin, white	12190401	1
Caelo	Paraffin, white	12209203	3
Caelo	Paraffin, white	122092004	1
Caelo	Paraffin, white	12209204	16
Großhandel	Paraffin, white	12209204	1
Caesar & Loretz GmbH, 4...	Paraffin, white	12209204	1
Anzag 27.12.12 ek:5.45	Paraffin, white	12209204	1
Anzag	Paraffin, white	12209204	1
Caelo	Paraffin, white	12209210	28
Noweda	Paraffin, white	12209210	1
Anzag 15.03.13 ek: 5,61EUR	Paraffin, white	12209210	1
Phönix	Paraffin, white	12209210	1
Caesar & Loretz GmbH, 4...	Paraffin, white	12209210	1
Pönix 19.04.2013	Paraffin, white	12209210	2
Cealo	Paraffin, white	12209210	1
Caelo	Paraffin, white	12306202	2
Caelo	Paraffin, white	12306302	5
Alliance Healthcare	Paraffin, white	12306302	1
Caelo	Paraffin, white	12306303	1
Caelo	Paraffin, white	12306401	4
Caelo	Paraffin, white	12311003	4
Caelo	Paraffin, white	1231010	1
Caelo	Paraffin, white	12311004	5
Gehe	Paraffin, white	12311004	1
Caelo	Paraffin, white	12311010	13
Sanacorp	Paraffin, white	12311010	1
Caelo	Paraffin, white	12311011	10
Caelo	Paraffin, white	12321902	1
Caelo	Paraffin, white	12321905	3
Caelo	Paraffin, white	12321906	4
Caelo	Paraffin, white	12321908	3
Caelo	Paraffin, white	12337701	8
Caelo	Paraffin, white	12337703	16
Caelo	Paraffin, white	12337704	11
Sanacorp	Paraffin, white	12337704	2
Caelo	Paraffin, white	12337706	14
Caesar & Loretz GmbH, 4...	Paraffin, white	12337706	1
Gehe am 27.2.14	Paraffin, white	12337706	1
Caelo	Paraffin, white	12337707	8
Noweda	Paraffin, white	12337707	1
Euro OTC	Paraffin, white	12337707	1
Caelo	Paraffin, white	12337708	12
Sanacorp	Paraffin, white	12337708	1

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Supplier	Substance	Batch	Spectra
Caesar&Loretz GmbH/Anzag	Paraffin, white	12337708	1
Caelo	Paraffin, white	12337709	12
Phoenix 18.03.2014	Paraffin, white	12337709	1
Caelo	Paraffin, white	12374501	5
Grokhhandel	Paraffin, white	12374502	1
Caelo	Paraffin, white	12374502	8
AHC 08.07.13 EK5,61	Paraffin, white	12374502	1
Caelo	Paraffin, white	1237706	1
Fagron	Paraffin, white	12B20-T02	1
Phönix 16.10.12	Paraffin, white	12D16-T01	1
Fagron	Paraffin, white	12D16-To1	1
Fagron	Paraffin, white	12D16-T01	2
Caelo	Paraffin, white	12D19-T54-000715	3
Fagron	Paraffin, white	12D19-T54-000715	1
Fagron	Paraffin, white	12H10-T05	2
Fagron	Paraffin, white	12I17-T01	2
Fagron	Paraffin, white	12J31-T52-000963	1
Fagron	Paraffin, white	12K01-T52	1
Fagron	Paraffin, white	12K01-T52-000717	1
Fagron	Paraffin, white	12K01-T52-002659	2
Caelo	Paraffin, white	12K01-T52-002659	1
Euro OTC	Paraffin, white	12K01-T52-002659	1
Caelo	Paraffin, white	13005701	9
Fagron	Paraffin, white	13/19-T05-006192	1
Fagron	Paraffin, white	13/19-T05-006193	1
Caelo	Paraffin, white	13005710	8
Caelo	Paraffin, white	13005711	11
Caelo	Paraffin, white	13005712	13
Caelo	Paraffin, white	13005713	4
Caelo	Paraffin, white	13005719	6
Caelo	Paraffin, white	13005720	2
Caelo	Paraffin, white	13011407	1
Euro OTC	Paraffin, white	1302022-01	8
Caelo	Paraffin, white	13031301	1
Caelo	Paraffin, white	13028302	1
Caelo	Paraffin, white	1305031-01	1
Euro OTC	Paraffin, white	1305031-01	5
Caelo	Paraffin, white	130510	1
Caelo	Paraffin, white	13051305	1
Caelo	Paraffin, white	13084902	14
Caelo	Paraffin, white	13084903	1
Caelo	Paraffin, white	13084905	12
Caesar/Noweda	Paraffin, white	13084905	1
Sanacorp	Paraffin, white	13084906	3
Caelo	Paraffin, white	13084906	11
Phoenix	Paraffin, white	13084906	1
Caelo	Paraffin, white	13084907	1
Caelo	Paraffin, white	13095601	8
canea, gehe	Paraffin, white	13095701	2
Caelo	Paraffin, white	13095701	2
Caesar & Loretz GmbH Hi...	Paraffin, white	13095701	1
Caelo	Paraffin, white	13109010	1
Caelo	Paraffin, white	1310909	1
Caelo	Paraffin, white	1310911	1
Caelo	Paraffin, white	13121303	1
gehe 215.08.2013	Paraffin, white	1313009	1
Caelo	Paraffin, white	13130901	6
Caelo	Paraffin, white	13130907	5
Caelo	Paraffin, white	13130909	11
Sanacorp	Paraffin, white	13130909	2

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Supplier	Substance	Batch	Spectra
gehe 30.09.13	Paraffin, white	13130909	1
Caesar & Loretz GmbH	Paraffin, white	13130909	1
Caelo	Paraffin, white	13130910	4
Caesar & Loretz GmbH, 4...	Paraffin, white	13130911	1
Caelo	Paraffin, white	13130911	8
Großhandel	Paraffin, white	13130911	1
Caelo	Paraffin, white	13130912	12
Caelo	Paraffin, white	13163602	2
Caelo	Paraffin, white	13163701	6
Caelo	Paraffin, white	13163702	3
Caelo	Paraffin, white	13174901	1
Caelo	Paraffin, white	13185502	7
Caelo	Paraffin, white	13185501	1
Caelo	Paraffin, white	13185504	5
Caelo	Paraffin, white	13185505	1
Caolo/Anzag	Paraffin, white	13185505	1
Caelo	Paraffin, white	13185506	3
Caelo	Paraffin, white	13185507	4
Caelo	Paraffin, white	13185512	6
Caelo	Paraffin, white	13185513	1
Caelo	Paraffin, white	13185514	2
Caelo	Paraffin, white	1326408	1
Caelo	Paraffin, white	13268408	17
Caelo	Paraffin, white	13268409	13
Caelo	Paraffin, white	13268410	9
Phönix	Paraffin, white	13268410	1
Caelo	Paraffin, white	13268411	5
Caelo	Paraffin, white	13268420	4
Sanacorp	Paraffin, white	13268420	1
Großhandel	Paraffin, white	13268421	1
Caelo	Paraffin, white	13268421	9
Noweda	Paraffin, white	13268421	1
Phoenix	Paraffin, white	13268423	1
Caelo	Paraffin, white	13333101	1
Caelo	Paraffin, white	13336702	2
Caelo	Paraffin, white	13338702	4
Noweda	Paraffin, white	13337706	1
Caelo	Paraffin, white	13338703	9
Phoenix am 10.03.2014	Paraffin, white	13338703	1
Fagron	Paraffin, white	13338703	1
Caelo	Paraffin, white	13338704	1
Caelo	Paraffin, white	13338707	7
Caelo	Paraffin, white	13338710	10
Berkel AHK	Paraffin, white	13338710	1
Sanacorp	Paraffin, white	13338712	1
Caelo	Paraffin, white	13338711	1
Caelo	Paraffin, white	13338712	5
Herbasinica	Paraffin, white	13338712	1
Caelo	Paraffin, white	13338713	3
Caelo	Paraffin, white	13338714	5
Caelo	Paraffin, white	13341602	3
Caelo	Paraffin, white	13341605	6
Phonix	Paraffin, white	13341604	1
Caelo	Paraffin, white	13341606	5
Caelo	Paraffin, white	13341608	7
Caelo	Paraffin, white	13341612	7
Caelo	Paraffin, white	13365103	2
Caelo	Paraffin, white	13365104	3
Caelo	Paraffin, white	13380702	3
Caelo	Paraffin, white	13380703	10

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Supplier	Substance	Batch	Spectra
Caelo	Paraffin, white	13380708	5
Caelo	Paraffin, white	13380707	5
Caelo	Paraffin, white	13380720	17
Caelo	Paraffin, white	13380721	8
Fagron	Paraffin, white	13D02-T02-002660	1
Caelo	Paraffin, white	13D02-T02-002660	1
Fagron	Paraffin, white	13D02-T02-004621	1
Fagron	Paraffin, white	13I19-T05-006192	2
Fagron	Paraffin, white	13I19-T05-008452	2
Fagron	Paraffin, white	13I19-T05-006193	1
Beiersdorf/Gehe	Paraffin, white	1401017-01	1
Euro OTC	Paraffin, white	1401017-01	1
Euro OTC	Paraffin, white	1401018-01	2
Fagron	Paraffin, white	1401453	1
Caelo	Paraffin, white	14025101	3
Caelo	Paraffin, white	14025201	9
Euro OTC	Paraffin, white	1405014-01	5
Bombastus	Paraffin, white	1406212549	1
Caelo	Paraffin, white	14081205	1
Caelo	Paraffin, white	14087402	4
Berkel AHK	Paraffin, white	14087403	1
Caelo	Paraffin, white	14087404	7
Caelo	Paraffin, white	14087405	3
Caelo	Paraffin, white	14087410	5
Caelo	Paraffin, white	14124704	6
Caelo	Paraffin, white	14124702	1
Phönix	Paraffin, white	14124703	1
Caelo	Paraffin, white	14124705	1
Caelo	Paraffin, white	14124706	2
Caelo	Paraffin, white	14124707	8
Caelo	Paraffin, white	14189006	6
Caelo	Paraffin, white	14189002	5
Caelo	Paraffin, white	14189018	5
Fagron	Paraffin, white	14189019	1
Caelo	Paraffin, white	14301804	4
Caelo	Paraffin, white	14201001	2
Caelo	Paraffin, white	14200901	4
Fagron	Paraffin, white	14201001	1
Caelo	Paraffin, white	14301805	2
Caelo	Paraffin, white	14324301	7
Fagron	Paraffin, white	14E30-T07-012095	1
Fagron	Paraffin, white	14J03-T03-020827	3
Fagron	Paraffin, white	14e30-t07-012095	1
Caelo	Paraffin, white	15031402	1
Fagron	Paraffin, white	14j03-to3-020827	1
Caelo	Paraffin, white	15041305	1
Caelo	Paraffin, white	15060003	9
Caelo	Paraffin, white	15050003	1
Caelo	Paraffin, white	15060008	2
Caelo	Paraffin, white	15060005	2
Caelo	Paraffin, white	15101308	1
Caelo	Paraffin, white	15060012	2
Caelo	Paraffin, white	15060014	7
Caelo	Paraffin, white	15081406	1
Caelo	Paraffin, white	15162503	4
Caelo	Paraffin, white	15162504	7
Caelo	Paraffin, white	15162507	6
Caelo	Paraffin, white	15162508	1
Caelo	Paraffin, white	15162512	2
Caelo	Paraffin, white	15204303	11

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Supplier	Substance	Batch	Spectra
Caelo	Paraffin, white	15204304	2
Caelo	Paraffin, white	15219903	3
Caelo	Paraffin, white	15278805	3
Caelo	Paraffin, white	15278804	2
Caelo	Paraffin, white	15330502	1
Caelo	Paraffin, white	15336809	4
Caelo	Paraffin, white	15339806	7
Caelo	Paraffin, white	15349708	4
Caelo	Paraffin, white	15349701	4
Caelo	Paraffin, white	15441501	2
Caelo	Paraffin, white	1544150	1
Caelo	Paraffin, white	16029211	7
Caelo	Paraffin, white	16029221	2
Caelo	Paraffin, white	16029213	1
Caelo	Paraffin, white	16061403	1
Caelo	Paraffin, white	16071306	1
Sanacorp	Paraffin, white	16AKD2	1
Caelo	Paraffin, white	17011309	1
Caelo	Paraffin, white	17081202	1
Caelo	Paraffin, white	18041315	1
Caelo	Paraffin, white	17121206	1
Caelo	Paraffin, white	19091308	1
Caelo	Paraffin, white	19071401	1
Caelo	Paraffin, white	20031303	1
Bombastus	Paraffin, white	2002312549	1
Phönix Gotha	Paraffin, white	200567	1
Caelo	Paraffin, white	20061206	1
Caelo	Paraffin, white	20081304	1
Bombastus	Paraffin, white	2014Q2549	1
Phönix Gotha	Paraffin, white	201387	1
Caelo	Paraffin, white	21101306	1
Caelo	Paraffin, white	20160812-4	1
Caelo	Paraffin, white	22111306	1
Caelo	Paraffin, white	22081206	1
Caelo	Paraffin, white	23051101	1
Caelo	Paraffin, white	22011401	1
Caelo	Paraffin, white	23051404	1
Caelo	Paraffin, white	23071202	1
Caelo	Paraffin, white	25021403	1
Caelo	Paraffin, white	250414002	1
Caelo	Paraffin, white	26061307	1
Caelo	Paraffin, white	26081409	1
Caelo	Paraffin, white	26091303	1
Caelo	Paraffin, white	26091406	1
Caelo	Paraffin, white	26101202	1
Caelo	Paraffin, white	26111203	1
Caelo	Paraffin, white	27021402	1
Bombastus	Paraffin, white	2704212549	1
Bombastus	Paraffin, white	270492	1
Bombastus	Paraffin, white	270553	2
Caelo	Paraffin, white	27061301	1
Bombastus	Paraffin, white	270831	1
Caelo	Paraffin, white	27091205	1
Caelo	Paraffin, white	27061401	1
Bombastus	Paraffin, white	270980	2
Bombastus	Paraffin, white	270981	1
Caelo	Paraffin, white	27121304	1
Alliance Healthcare	Paraffin, white	276088	1
Bombastus	Paraffin, white	276088	2
Phoenix am 22.04.2014	Paraffin, white	270981	1

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Supplier	Substance	Batch	Spectra
Caelo	Paraffin, white	276127	1
Bombastus	Paraffin, white	276968	1
Bombastus	Paraffin, white	276127	1
Bombastus	Paraffin, white	277059	2
Bombastus	Paraffin, white	2761127	1
Gehe	Paraffin, white	277059	2
Bombastus	Paraffin, white	277060	4
Alliance Healthcare	Paraffin, white	277444	1
Bombastus	Paraffin, white	277986	2
Phönix	Paraffin, white	277986	1
Bombastus	Paraffin, white	277987	5
Phönix	Paraffin, white	277987	1
Caelo	Paraffin, white	277987	1
Bombastus	Paraffin, white	277988	2
Gehe 02.07.2013	Paraffin, white	277988	2
Bombastus	Paraffin, white	278595	1
Bombastus	Paraffin, white	278620	1
Gehe	Paraffin, white	279161	1
Bombastus	Paraffin, white	279161	5
Bombastus	Paraffin, white	279805	1
Bombastus	Paraffin, white	279969	5
Gehe	Paraffin, white	279969	1
Bombastus	Paraffin, white	279970	3
AHD, 30.09.2013	Paraffin, white	279970	1
Bombstus/ Phönix	Paraffin, white	280451	1
Bombastus	Paraffin, white	280452	6
Phönix	Paraffin, white	280451	1
Caelo	Paraffin, white	280702	1
Bombastus	Paraffin, white	281291	3
Bombastus	Paraffin, white	280702	1
Phönix	Paraffin, white	281291	1
Bombastus	Paraffin, white	281539	1
Bombastus	Paraffin, white	282336	1
Bombastus	Paraffin, white	282700	3
Bombastus	Paraffin, white	282699	1
Caelo	Paraffin, white	282700	1
Bombastu-Werke AG/Gehe	Paraffin, white	282964	3
Caelo	Paraffin, white	282964	1
Bombastus	Paraffin, white	282966	6
Gehe	Paraffin, white	282966	1
Bombastus	Paraffin, white	283873	1
Bombastus	Paraffin, white	283949	6
Bombastus	Paraffin, white	283948	1
Caelo	Paraffin, white	283949	1
Bombastus	Paraffin, white	283951	1
Bombastus	Paraffin, white	285231	2
Bombastus	Paraffin, white	285309	1
Bombastus	Paraffin, white	285310	8
Bombastus	Paraffin, white	286095	3
Caelo	Paraffin, white	286095	1
Bombastus	Paraffin, white	286096	5
Gehe	Paraffin, white	286096	2
Bombastus	Paraffin, white	287149	2
Bombastus	Paraffin, white	287147	1
Caelo	Paraffin, white	29051201	1
Bombastus	Paraffin, white	302037	3
Bombastus	Paraffin, white	2909212549	1
Bombastus	Paraffin, white	3013M2549	1
Bombastus	Paraffin, white	30061201	1
Bombastus	Paraffin, white	4013E-02549	1

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Supplier	Substance	Batch	Spectra
Bombastus	Paraffin, white	3113Q02549	1
Henry Lamotte Oils GmbH	Paraffin, white	5098800	2
Caelo	Paraffin, white	5098800	1
HerryLamotte/AHD	Paraffin, white	5098800	1
Bombastus	Paraffin, white	5213A2549	1
Phönix, 30.10.2012	Paraffin, white	5322600	1
Bombastus	Paraffin, white	5215200	1
Henry Lamotte Oils GmbH	Paraffin, white	5322600	1
Lamotte	Paraffin, white	5215200	1
Anzag/Lamotte	Paraffin, white	5322600	1
Henry Lamotte Oils GmbH	Paraffin, white	5489700	3
Phönix	Paraffin, white	5489700	1
Lamotte	Paraffin, white	5322600	1
AHD	Paraffin, white	5489700	1
gehe 26.11.13	Paraffin, white	5489700	1
Gehe am 03.02.2014	Paraffin, white	5489700	1
Henry Lamotte Oils GmbH	Paraffin, white	5538300	2
wolff/AHD	Paraffin, white	5538300	1
henry lamotte oils gmbh	Paraffin, white	5538300	1
Lamotte/ Anzag	Paraffin, white	5538300	1
Henry Lamotte GMBH/AHD	Paraffin, white	5691100	2
Henry Lamotte Oils GmbH	Paraffin, white	5691100	1
Henry Lamotte Oils GmbH	Paraffin, white	6000083007	2
Bombastus	Paraffin, white	60081102	1
Caelo	Paraffin, white	AKD50	1
Euro OTC	Paraffin, white	929392	1
Caelo	Paraffin, white	jjjjjj	1
Herbasinica	Paraffin, white		2
Euro OTC	Paraffin, white	F602635	1
Euro OTC	Paraffin, white	F603290	1
Phagron	Paraffin, white		1
Caelo	Paraffin, white	50115/1	1
Caelo	Paraffin, white	4051502	1
Caelo	Paraffin, white	5121403	1
Fagron	Paraffin, white	probe	1
Caelo	Paraffin, white	7031502	1
Caelo	Paraffin, white	11021510	1
Caelo	Paraffin, white	133380703	1
Caelo	Paraffin, white	13380704	5
cae	Paraffin, white	13380706	1
Caelo	Paraffin, white	13380706	3
Sanacorp	Paraffin, white	13380707	1
Sanacorp	Paraffin, white	13380709	1
Caelo	Paraffin, white	13380709	4
Caelo	Paraffin, white	13380719	4
Fagron	Paraffin, white	13h19-T05-008453	1
Phönix Gotha	Paraffin, white	14087402	1
Caelo	Paraffin, white	14087406	2
Caelo	Paraffin, white	14087409	1
Fagron	Paraffin, white	14124703	1
Cealo	Paraffin, white	14124707	1
Caelo	Paraffin, white	14124708	3
Caelo	Paraffin, white	14189003	2
Caelo	Paraffin, white	14189004	1
Caelo	Paraffin, white	14189007	4
Caelo	Paraffin, white	14248403	1
Caelo	Paraffin, white	14324601	2
Caelo	Paraffin, white	14347302	9
Fagron	Paraffin, white	14E30-T07	2
Fagron	Paraffin, white	14E30-T07-012096	4

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Supplier	Substance	Batch	Spectra
Fagron	Paraffin, white	14E30-T07-014285	4
Fagron	Paraffin, white	14j03-t003-020827	1
Caelo	Paraffin, white	15050004	1
Caelo	Paraffin, white	15050005	1
Caelo	Paraffin, white	15060006	4
Phönix Gotha	Paraffin, white	15060012	1
Caelo	Paraffin, white	15121407	1
Caelo	Paraffin, white	17101410	1
Caelo	Paraffin, white	18041504	1
Caelo	Paraffin, white	20061503	1
Caelo	Paraffin, white	21051509	1
Caelo	Paraffin, white	20031518	1
Caelo	Paraffin, white	22011510	1
Caelo	Paraffin, white	28041508	1
Caelo	Paraffin, white	22111401	1
Bombastus	Paraffin, white	287148	2
Bombastus	Paraffin, white	288714	2
Bombastus	Paraffin, white	288715	1
Gehe	Paraffin, white	288714	2
Bombastus	Paraffin, white	288716	4
Bombastus	Paraffin, white	288717	3
Bombastus	Paraffin, white	2888717	1
Phönix Gotha	Paraffin, white	289344	1
Bombastus	Paraffin, white	289344	1
Bombastus	Paraffin, white	290271	4
Fagron	Paraffin, white	290441	1
Caelo	Paraffin, white	290441	2
Bombastus	Paraffin, white	290441	4
Bombastus	Paraffin, white	291318	9
Bombastus	Paraffin, white	290714	2
Bombastus	Paraffin, white	292219	1
Bombastus	Paraffin, white	292220	1
Bombastus	Paraffin, white	295301	4
Bombastus	Paraffin, white	300120	4
Bombastus	Paraffin, white	297282	1
Caelo	Paraffin, white	30121427	1
Euro OTC	Paraffin, white	5691100	1
Sanacorp	Paraffin, white		1
Sanacorp	Paraffin, white	107/AKD6	1
Caelo	Paraffin, white	4091517	1
Sanacorp	Paraffin, white	106/AKD4	1
Caelo	Paraffin, white	12081504	1
Bombastus	Paraffin, white	12/2019	1
Caelo	Paraffin, yellow	12306302	1
Euro OTC	Paraffin, yellow	12321908	1
Gehe 20.06.15/euro	Paraffin, white	13380709	1
Noweda	Paraffin, white	13380721	1
Caelo	Paraffin, white	14092015B	1
Caelo	Paraffin, yellow	14248403	2
Caelo	Paraffin, yellow	14324301	4
Caesar&Loretz/Noweda	Paraffin, yellow	14324301	1
Phönix	Paraffin, yellow	14324301	1
Caelo	Paraffin, yellow	14324501	4
Caelo	Paraffin, yellow	14324402	1
Caesar & Loretz GmbH Hi...	Paraffin, yellow	14324601	1
Caelo	Paraffin, yellow	14324601	1
Caelo	Paraffin, yellow	1432501	1
Caelo	Paraffin, white	14355806	5
Fagron	Paraffin, white	14I03-T03-020831	1
Fagron	Paraffin, white	14J03-T03-020831	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Paraffin, yellow	1503036-01	4
Euro OTC	Paraffin, white	1501037-01	1
Eurho/Noweda	Paraffin, white	1501037-01	1
Caelo	Paraffin, white	15050002	1
Euro OTC	Paraffin, white	1505017-01	3
Caelo	Paraffin, white	15060004	3
Hedinger	Paraffin, white	15060004	1
Caelo	Paraffin, white	15060007	2
Caelo	Paraffin, white	15060013	2
Anzag/Henry Lamotte	Paraffin, white	15060014	1
Euro OTC	Paraffin, white	150901901	1
Euro OTC	Paraffin, white	1509019-01	1
Caelo	Paraffin, white	15162501	2
Ebert & Jacobi 19.07...	Paraffin, white	1509019-01	1
Caelo	Paraffin, white	15162505	6
Caelo	Paraffin, white	15162519	1
Caelo	Paraffin, white	15204301	1
Caelo	Paraffin, white	15204302	5
Caelo	Paraffin, yellow	15219903	4
Caesar & Loretz/Noweda	Paraffin, yellow	15330401	1
Caelo	Paraffin, yellow	15330401	3
Noweda	Paraffin, yellow	15330402	1
Caelo	Paraffin, yellow	15330402	1
Caelo	Paraffin, yellow	15330502	1
Caelo	Paraffin, yellow	15330601	2
Caelo	Paraffin, white	15336808	1
Caelo	Paraffin, white	15336810	2
Caelo	Paraffin, white	15339805	2
Noweda	Paraffin, white	15339806	1
Euro OTC	Paraffin, white	15339806	1
Caesar & Loretz/Noweda	Paraffin, white	15339806	1
Caelo	Paraffin, white	15339807	5
Caelo	Paraffin, white	15339808	6
Caesar & Loretz	Paraffin, white	15339808	1
Caelo	Paraffin, white	15349702	1
Caelo	Paraffin, white	15349706	1
Phoenix	Paraffin, white	15349706	1
Caelo	Paraffin, white	15349707	1
Caelo	Paraffin, white	15349709	3
Euroo/Gehe	Paraffin, white	1602009-01	1
Euro OTC	Paraffin, white	1602009-01	2
Phoenix	Paraffin, white	16029210	1
Caelo	Paraffin, white	16029210	1
Caelo	Paraffin, white	16029222	1
Caelo	Paraffin, white	16029212	1
Caelo	Paraffin, white	16029219	1
Noweda	Paraffin, yellow	16032502	1
Phönix	Paraffin, yellow	16032602	1
Caelo	Paraffin, yellow	16032602	2
Sanacorp, 21.07.2016	Paraffin, white	1605019-01	2
Caelo	Paraffin, yellow	16032603	1
Euro OTC	Paraffin, white	1605019-01	2
Caelo	Paraffin, white	16138003	3
Caelo	Paraffin, white	161338003	1
Noweda	Paraffin, white	16138004	1
Caelo	Paraffin, white	16138004	1
Caelo	Paraffin, white	16181901	1
Caelo	Paraffin, white	16181902	1
Caelo	Paraffin, white	16181903	1
PHÖNIX	Paraffin, white	16227402	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH Hi...	Paraffin, white	16227403	1
Caelo	Paraffin, yellow	17082015E	1
Caelo	Paraffin, white	16227403	1
Caelo	Paraffin, white	20071505	1
Caelo	Paraffin, yellow	28071509	1
Bombastus	Paraffin, yellow	28270	1
Bombastus	Paraffin, white	293553	1
Bombastus	Paraffin, white	291319	1
Bombastus	Paraffin, white		1
Bombastus	Paraffin, yellow	293629	2
Bombastus	Paraffin, white	294852	1
Caelo	Paraffin, white	295300	1
Bombastus	Paraffin, white	295265	2
Bombastus	Paraffin, yellow	296654	4
Euro OTC	Paraffin, white	297283	1
Bombastus	Paraffin, white	297283	5
Bombastus	Paraffin, white	298599	4
Bombastus	Paraffin, white	299469	2
Bombastus	Paraffin, white	2999469	1
Bombastus	Paraffin, yellow	300423	1
Bombastus	Paraffin, yellow	301908	2
Bombastus	Paraffin, white	304124	2
Sanacorp	Paraffin, yellow	57/AKD4	1
Caelo	Paraffin, white	6000083007	1
Caelo	Paraffin, white	6002062001	1
Caelo	Paraffin, white	14189008	1
Caelo	Paraffin, white	14201003	1
Beiersdorf AG	Eye paraffin	15441502	1
Caelo	Paraffin, white	16227405	1
Bombastus	Paraffin, white	267671	2
GEHE	Paraffin, white	270163	1
GEHE	Paraffin, white	270834	1
Bombastus	Paraffin, white	270984	1
Caelo	Paraffin, white	12081502	1
Caelo	Paraffin, white	1210006-01	1
Gehe	Paraffin, white	1210006-01	1
Caelo	Paraffin, white	1215106	2
Sanacorp	Paraffin, white	12374502	1
Gutenberg-Apotheke	Paraffin, white	13185502	1
Gehe	Paraffin, white	277060	1
Bombastus	Paraffin, white	282964	1
Caelo	Paraffin, white	51210195	1
Henry Lamotte/N/14.12.12	Paraffin, white	5322600	1
Fagron	Paraffin, white	790619-013771	1
Caelo	Paraffin, white	P159/14	1
GEHE	Paraffin	12102101	1
Ichtyol, Noweda	Fatty ointment anhydrous, wa...	12A147	1
Beiersdorf / Noweda	Wool alcohol ointment DAB	414610	1
Apomix/Noweda	Wool alcohol ointment SR wit...	1A180215	1
Caelo	Wool alcohol ointment DAB	4067201	1
Caelo	Wool alcohol ointment DAB	4051505	1
Apomix	Wool alcohol ointment SR wit...	5231213	1
Henry Lamotte Oels GmbH	Wool alcohol ointment SR wit...	7A111214	2
Defektur	Wool alcohol ointment DAB	10/15	1
Euro OTC	Wool alcohol ointment DAB	1204030-01	1
Eurho/Noweda	Wool alcohol ointment DAB	1211017-01	1
Caelo	Wool alcohol ointment DAB	13067103	4
Ebert	Wool alcohol ointment DAB	13242602	1
Caelo	Wool alcohol ointment DAB	13242902	6
Caelo	Wool alcohol ointment DAB	1324602	1

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Supplier	Substance	Batch	Spectra
Caelo	Wool alcohol ointment DAB	1325501	1
DAB 2008	Wool alcohol ointment DAB	13255101	1
Caelo	Wool alcohol ointment SR wit...	13264102	2
Caele/ Jenne	Wool alcohol ointment SR wit...	13340003	1
Fagron	Wool alcohol ointment DAB	13D09-T04	1
Caelo	Wool alcohol ointment SR wit...	14032502	1
Caelo	Wool alcohol ointment DAB	14022902	1
Caelo	Wool alcohol ointment DAB	14067001	4
Phönix	Wool alcohol ointment DAB	14067001	1
Caelo	Wool alcohol ointment DAB	1406701	1
Caelo	Wool alcohol ointment DAB	14067101	3
Berkel AHK	Wool alcohol ointment DAB	14067201	1
Caelo	Wool alcohol ointment DAB	14067301	1
Caelo	Wool alcohol ointment DAB	14067401	2
Caelo	Wool alcohol ointment DAB	14152803	1
Caelo	Wool alcohol ointment DAB	14152902	1
Phoenix	Wool alcohol ointment DAB	14153101	1
Caelo	Wool alcohol ointment DAB	14153601	5
Fagron	Wool alcohol ointment DAB	14153601	1
Caelo	Wool alcohol ointment DAB	14207702	1
Caelo	Wool alcohol ointment DAB	14283001	12
Caesar & Loretz GmbH Hi...	Wool alcohol ointment DAB	14283001	1
Caelo	Wool alcohol ointment DAB	14283102	9
Caelo	Wool alcohol ointment DAB	14283103	7
Caelo	Wool alcohol ointment DAB	1428801	1
Fagron	Wool alcohol ointment DAB	14H19-T01-011354	1
Alliance Health 30.10.2...	Wool alcohol ointment DAB	14H19-T02-011354	1
Fagron	Wool alcohol ointment DAB	14H19-T02-018184	1
Fagron	Wool alcohol ointment DAB	14H19-T02-011354	1
Fagron	Wool alcohol ointment DAB	14H19T02018184	1
Caelo	Wool alcohol ointment DAB	15035301	5
Caelo	Wool alcohol ointment DAB	15035501	3
Caelo	Wool alcohol ointment SR wit...	15047002	2
Caelo	Wool alcohol ointment SR wit...	15047101	1
Caelo	Wool alcohol ointment DAB	15225501	3
P.W. Beyvers GmbH/Phönix	Wool alcohol ointment DAB	15225501	3
Caelo	Wool alcohol ointment DAB	15225601	6
Phönix Gotha	Wool alcohol ointment DAB	15225601	1
caesar&lorenz,Phönix	Wool alcohol ointment DAB	15225601	1
Caelo	Wool alcohol ointment DAB	1522802	1
Caelo	Wool alcohol ointment DAB	15228202	6
Noweda	Wool alcohol ointment DAB	15361801	1
Caelo	Wool alcohol ointment DAB	15361901	4
Caelo	Wool alcohol ointment DAB	15362001	8
Caelo	Wool alcohol ointment DAB	15362002	5
Caesar&Loretz GmbH	Wool alcohol ointment DAB	15362002	1
Caelo	Wool alcohol ointment DAB	15362003	1
Fagron	Wool alcohol ointment DAB	15E18-20-021463	1
Fagron	Wool alcohol ointment DAB	15E18-T20-021463	1
Bombastus	Wool alcohol ointment DAB	16007201	2
Caelo	Wool alcohol ointment DAB	16066501	1
Caelo	Wool alcohol ointment DAB	16066601	2
Caelo	Wool alcohol ointment DAB	16066801	1
Caelo	Wool alcohol ointment DAB	16066701	1
Caelo	Wool alcohol ointment DAB	16198501	3
Caesar & Loretz	Wool alcohol ointment DAB	16198401	1
Caelo	Wool alcohol ointment DAB	16298502	1
Defektur	Wool alcohol ointment DAB	18/14	1
Caelo	Wool alcohol ointment DAB	21051510	1
GEHE 17.06.2014	Wool alcohol ointment DAB	23033310	1

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Supplier	Substance	Batch	Spectra
Pharmachem	Wool alcohol ointment SR wit...	250116	1
Caelo	Wool alcohol ointment DAB	259166	1
Defektur	Wool alcohol ointment DAB	26/14	1
Bombastus	Wool alcohol ointment DAB	277024	2
Gehe	Wool alcohol ointment SR wit...	279105	2
Bombastus	Wool alcohol ointment DAB	280061	1
Bombastus	Wool alcohol ointment SR wit...	283174	1
Bombastus	Wool alcohol ointment DAB	283176	1
Bombastus	Wool alcohol ointment DAB	283618	5
gehe	Wool alcohol ointment DAB	284378	1
Phönix Gotha	Wool alcohol ointment SR wit...	284381	1
Bombastus	Wool alcohol ointment SR wit...	284378	1
Bombastus	Wool alcohol ointment DAB	285423	1
Apomix	Wool alcohol ointment DAB	285950	1
Caelo	Wool alcohol ointment DAB	286882	1
Bombastus	Wool alcohol ointment SR wit...	286884	1
Phönix Gotha	Wool alcohol ointment DAB	286884	1
Noweda	Wool alcohol ointment DAB	287013	1
Bombastus	Wool alcohol ointment DAB	287013	2
Gehe	Wool alcohol ointment SR wit...	288687	1
Phönix Gotha	Wool alcohol ointment DAB	288688	1
Bombastus	Wool alcohol ointment DAB	288688	1
Bombastus	Wool alcohol ointment DAB	288766	1
Bombastus	Wool alcohol ointment DAB	288834	6
UNISAN	Wool alcohol ointment DAB	289509	1
Bombastus	Wool alcohol ointment DAB	289509	3
Gehe	Wool alcohol ointment DAB	289510	1
Caelo	Wool alcohol ointment DAB	291175	1
Bombastus	Wool alcohol ointment SR wit...	291176	1
Bombastus	Wool alcohol ointment DAB	291796	2
Bombastus	Wool alcohol ointment DAB	291797	1
Bombastus	Wool alcohol ointment DAB	293091	1
Bombastus	Wool alcohol ointment DAB	293092	1
Caelo	Wool alcohol ointment DAB	293093	1
Bombastus	Wool alcohol ointment SR wit...	293378	1
Bombastus	Wool alcohol ointment DAB	293956	8
Bombastus	Wool alcohol ointment SR wit...	295359	1
Bombastus	Wool alcohol ointment SR wit...	295358	1
Bombastus	Wool alcohol ointment DAB	296235	1
Bombastus	Wool alcohol ointment DAB	296435	6
Bombastus	Wool alcohol ointment SR wit...	297125	1
Bombastus	Wool alcohol ointment SR wit...	297128	1
Bombastus	Wool alcohol ointment SR wit...	297130	1
Bombastus	Wool alcohol ointment DAB	298577	5
Bombastus	Wool alcohol ointment DAB	298578	1
Bombastus	Wool alcohol ointment SR wit...	300083	1
Bombastus	Wool alcohol ointment DAB	300281	1
Bombastus	Wool alcohol ointment DAB	300282	1
Bombastus	Wool alcohol ointment DAB	301200	1
Bombastus	Wool alcohol ointment SR/DAC	301938	1
Bombastus	Wool alcohol ointment DAB	302206	6
Bombastus	Wool alcohol ointment DAB	303846	3
Bombastus	Wool alcohol ointment DAB	305879	2
Beiersdorf/ Sanacorp	Wool alcohol ointment DAB	34344210	1
Beiersdorf/Gehe	Wool alcohol ointment DAB	34554710	1
Noweda / Beiersdorf AG	Wool alcohol ointment DAB	34424610	1
Defektur	Wool alcohol ointment DAB	38/14	1
Baiersdorf AG	Wool alcohol ointment DAB	40726610	1
Gehe/Beiersdorf	Wool alcohol ointment DAB	40726610	1
Beiersdorf/ Gehe	Wool alcohol ointment DAB	40916810	1

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Supplier	Substance	Batch	Spectra
Fagron	Wool alcohol ointment DAB	40956810	1
Defektur	Wool alcohol ointment DAB	41/14	1
Caelo	Wool alcohol ointment DAB	41047010	1
Beiersdorf	Wool alcohol ointment DAB	41910710	1
Beiersdorf / Noweda	Wool alcohol ointment DAB	41910710	1
Caesar & Loretz GmbH	Wool alcohol ointment DAB	41930610	1
Gehe/Beiersdorf	Wool alcohol ointment DAB	41930610	2
Phönix Gotha	Wool alcohol ointment DAB	41930610	1
Beiersdorf/Gehe	Wool alcohol ointment DAB	41940610	2
Caelo	Wool alcohol ointment DAB	41940610	1
Beiersdorf / E	Wool alcohol ointment DAB	41940610	1
Phoenix	Wool alcohol ointment DAB	41940610	1
Gehe	Wool alcohol ointment DAB	41950710	1
Defektur	Wool alcohol ointment DAB	42/14	1
Beiersdorf/Anzag	Wool alcohol ointment DAB	42531910	1
Beiersdorf/Gehe	Wool alcohol ointment DAB	43142910	1
Sanacorp	Wool alcohol ointment DAB	44/AKD10	1
Beiersdorf/ Sanacorp	Wool alcohol ointment DAB	44824310	1
Defektur	Wool alcohol ointment DAB	45/14	1
Beiersdorf/ Nowea	Wool alcohol ointment DAB	45054410	1
Defektur	Wool alcohol ointment DAB	5/15	1
Beiersdorf/ Gehe	Wool alcohol ointment DAB	50414810	1
Gehe	Wool alcohol ointment DAB	50444710	1
Beiersdorf / Noweda	Wool alcohol ointment DAB	50444710	1
Beiersdorf/Noweda	Wool alcohol ointment DAB	50815310	1
Gehe/Beiersdorf	Wool alcohol ointment DAB	50815310	1
Caelo	Wool alcohol ointment DAB	50835210	1
Beiersdorf/N	Wool alcohol ointment DAB	50845210	1
Noweda	Wool alcohol ointment DAB	50845210	1
Beiersdorf AG	Wool alcohol ointment DAB	50845210	1
Beiersdorf/Phoenix	Wool alcohol ointment DAB	50845210	1
Beiersdorf / Noweda	Wool alcohol ointment DAB	50845210	1
Beiersdorf/Phoenix	Wool alcohol ointment DAB	50935410	1
Beiersdorf/N	Wool alcohol ointment DAB	51015610	1
Fagron	Wool alcohol ointment DAB	53437010	1
Beiersdorf über Phoenix	Wool alcohol ointment DAB	53437010	1
Beiersdorf/Noweda	Wool alcohol ointment DAB	54127710	1
Bayersdorf	Wool alcohol ointment DAB	54137710	1
Beiersdorf/Sanacorp	Wool alcohol ointment DAB	54157810	1
Henry Lamotte Oils GmbH	Wool alcohol ointment DAB	5860600	1
Bombastus	Wool alcohol ointment DAB	60080202	1
Bombastus	Wool alcohol ointment DAB	60080203	1
Beiersdorf AG	Wool alcohol ointment DAB	60419110	1
Beiersdorf/Phoenix	Wool alcohol ointment DAB	60539210	1
Beiersdorf/Sanacorp	Wool alcohol ointment DAB	60539210	1
Beiersdorf/AHD	Wool alcohol ointment DAB	61149910	1
Phönix	Wool alcohol ointment DAB	61149910	1
PHÖNIX	Wool alcohol ointment DAB	63052310	1
Bombastus	Wool alcohol ointment DAB	251850	1
Bombastus	Wool alcohol ointment DAB	252186	1
Bombastus	Wool alcohol ointment DAB	256518	1
Bombastus	Wool alcohol ointment DAB	261436	1
Bombastus	Wool alcohol ointment DAB	262037	1
Bombastus	Wool alcohol ointment DAB	263456	1
Bombastus	Wool alcohol ointment DAB	265502	1
Bombastus	Wool alcohol ointment DAB	266204	1
Bombastus	Wool alcohol ointment DAB	267675	3
Noweda	Wool alcohol ointment DAB	267675	1
Gehe	Wool alcohol ointment DAB	268470	1
DAC 2011	Wool alcohol ointment DAB	268471	1

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Supplier	Substance	Batch	Spectra
Bombastus	Wool alcohol ointment DAB	270640	2
Bombastus	Wool alcohol ointment DAB	270642	3
phönix 22.01.2013	Wool alcohol ointment DAB	270642	1
Noweda	Wool alcohol ointment DAB	270642	2
Phönix	Wool alcohol ointment SR wit...	270781	1
Bombastus	Wool alcohol ointment DAB	270780	1
Bombastus	Wool alcohol ointment SR wit...	270781	1
Bombastus	Wool alcohol ointment SR wit...	270784	2
Bombastus	Wool alcohol ointment DAB	272171	1
Bombastus	Wool alcohol ointment DAB	274282	1
Sanacorp	Wool alcohol ointment DAB	274283	1
Defektur	Wool alcohol ointment DAB	2/13	1
Apomix/Noweda	Wool alcohol ointment SR wit...	2A080713	1
Phönix Gotha	Wool alcohol ointment DAB	34554710	1
Defektur	Wool alcohol ointment DAB	3/14	1
Caelo	Wool alcohol ointment DAB	4061204	1
Gehe 02.07.2013	Wool alcohol ointment DAB	4352610	1
Defektur	Wool alcohol ointment DAB	6/14	1
Caelo	Wool alcohol ointment DAB	7121202	1
Beiersdorf/ Phoenix	Wool alcohol ointment DAB	814Q1270	1
Beiersdorf/ Phoenix	Wool alcohol ointment DAB	814Q1370	1
Pharmachem/Phönix	Wool alcohol ointment DAB	90812	1
Caelo	Wool alcohol ointment DAB	11068001	1
Euro OTC	Wool alcohol ointment DAB	1108057-01	4
Euro OTC	Wool alcohol ointment DAB	110805701	1
Caelo	Wool alcohol ointment DAB	11184901	1
Kehr	Wool alcohol ointment DAB	11184901	1
Caelo	Wool alcohol ointment DAB	11184902	1
Caelo	Wool alcohol ointment DAB	11185001	1
Caesar & Loretz GmbH 40...	Wool alcohol ointment DAB	11185101	1
Caelo	Wool alcohol ointment DAB	11185201	1
Caelo	Wool alcohol ointment DAB	11232902	1
Kehr	Wool alcohol ointment DAB	11335001	1
Caelo	Wool alcohol ointment DAB	11335001	2
Gehe	Wool alcohol ointment DAB	11335003	1
Caelo	Wool alcohol ointment DAB	11335003	1
Phönix Gotha	Wool alcohol ointment DAB	11335003	2
Klenk	Wool alcohol ointment DAB	11335101	1
Anzag	Wool alcohol ointment DAB	11335101	1
Caelo	Wool alcohol ointment DAB	11335101	6
Caelo	Wool alcohol ointment DAB	11335201	1
Kehr	Wool alcohol ointment DAB	1135001	1
Caelo	Wool alcohol ointment DAB	12016202	3
Caelo	Wool alcohol ointment DAB	12016203	8
Caelo	Wool alcohol ointment DAB	12076601	3
Anzag Ek: 3,24EUR 11.09.12	Wool alcohol ointment DAB	12076601	1
Caelo	Wool alcohol ointment DAB	12076602	1
Caelo	Wool alcohol ointment DAB	12076701	2
Caelo	Wool alcohol ointment SR wit...	12078201	1
Noweda	Wool alcohol ointment SR wit...	12078301	1
Noweda	Wool alcohol ointment SR wit...	12078201	1
Euro OTC	Wool alcohol ointment DAB	1211018-01	1
Erika Apotheke	Wool alcohol ointment DAB	1215001	1
Caelo	Wool alcohol ointment DAB	12151801	2
Caelo	Wool alcohol ointment DAB	12151802	2
Caelo	Wool alcohol ointment DAB	12151901	8
Caelo	Wool alcohol ointment DAB	12151903	5
Bombastus	Wool alcohol ointment DAB	12151903	1
Phönix Gotha	Wool alcohol ointment DAB	12152001	2
Noweda	Wool alcohol ointment SR wit...	12244302	1

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Supplier	Substance	Batch	Spectra
Caelo	Wool alcohol ointment DAB	12339901	4
Caelo	Wool alcohol ointment DAB	12340001	3
Caelo	Wool alcohol ointment DAB	12340002	4
Caelo	Wool alcohol ointment DAB	12340003	1
Caesar & Loretz GmbH	Wool alcohol ointment DAB	12340003	1
Caelo	Wool alcohol ointment DAB	1234002	1
fragon	Wool alcohol ointment DAB	12345	2
Caelo	Wool alcohol ointment DAB	13066903	1
A.H. 05.06.13 ek: 3,33EUR	Wool alcohol ointment DAB	13067101	1
Caelo	Wool alcohol ointment DAB	13067101	2
Hustadt Apotheke	Wool alcohol ointment DAB	13067102	1
Caelo	Wool alcohol ointment DAB	13067201	10
Caelo	Wool alcohol ointment SR wit...	13077301	2
Caelo	Wool alcohol ointment SR wit...	13077302	1
Caelo	Wool alcohol ointment DAB	13093202	1
Alliance Healthcare	Wool alcohol ointment DAB	13114001	1
Caelo	Wool alcohol ointment DAB	13114103	4
Caelo	Wool alcohol ointment DAB	13126001	6
Gehe	Wool alcohol ointment DAB	13126001	1
Caelo	Wool alcohol ointment DAB	13126101	1
Caelo	Wool alcohol ointment DAB	13242401	1
Caelo	Wool alcohol ointment DAB	13355202	1
Caelo	Wool alcohol ointment DAB	1367101	1
Fagron	Wool alcohol ointment DAB	13D09-T04-003308	5
Fagron	Wool alcohol ointment DAB	13D09T04003308	2
Beiersdorf	Wool alcohol ointment DAB	14349010	1
Beiersdorf AG	Wool alcohol ointment DAB	14549310	1
Fagron	Wool alcohol ointment DAB	14819510	1
Caelo	Wool alcohol ointment DAB	20061204	1
Caelo	Wool alcohol ointment DAB	20271211-1	1
Beiersdorf	Wool alcohol ointment DAB	20271211-3	1
Beiersdorf AG	Wool alcohol ointment DAB	21111310	1
Beiersdorf / K	Wool alcohol ointment DAB	22142410	1
Beiersdorf/Gehe	Wool alcohol ointment DAB	22412510	1
Gehe	Wool alcohol ointment DAB	22532710	1
Caelo	Wool alcohol ointment DAB	22532810	1
Beiersdorf AG	Wool alcohol ointment DAB	22532810	1
Beiersdorf/Otto	Wool alcohol ointment DAB	23033310	1
Gehe	Wool alcohol ointment DAB	23033310	1
Noweda	Wool alcohol ointment DAB	23223410	1
Beiersdorf/Gehe	Wool alcohol ointment DAB	23223410	1
Phönix	Wool alcohol ointment DAB	23733710	1
Caelo	Wool alcohol ointment DAB	25051306	1
Caelo	Wool alcohol ointment DAB	24655410	1
Bombastus	Wool alcohol ointment SR wit...	270776	1
Bombastus	Wool alcohol ointment SR wit...	274517	1
Bombastus	Wool alcohol ointment SR wit...	274518	3
Bombastus	Wool alcohol ointment DAB	275999	3
Phönix	Wool alcohol ointment DAB	275999	1
Bombastus	Wool alcohol ointment SR wit...	276135	1
Bombastus	Wool alcohol ointment SR wit...	277023	1
Gehe	Wool alcohol ointment DAB	277023	1
Bombastus	Wool alcohol ointment SR wit...	277024	3
Gehe	Wool alcohol ointment DAB	277191	2
Bombastus	Wool alcohol ointment DAB	277190	1
Bombastus	Wool alcohol ointment DAB	277191	1
Bombastus	Wool alcohol ointment DAB	277192	2
Bombastus	Wool alcohol ointment DAB	278684	2
Bombastus	Wool alcohol ointment SR wit...	279104	1
Bombastus	Wool alcohol ointment SR wit...	279105	1

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Supplier	Substance	Batch	Spectra
Bombastus	Wool alcohol ointment DAB	279934	3
Bombastus	Wool alcohol ointment SR wit...	280060	1
Bombastus	Wool alcohol ointment SR wit...	280058	1
Gehe	Wool alcohol ointment DAB	280061	2
Bombastus	Wool alcohol ointment SR wit...	280061	2
Phoenix	Wool alcohol ointment DAB	283619	1
Bombastus	Wool alcohol ointment DAB	300283	1
Caelo	Wool alcohol ointment DAB	30111302	1
Beiersdorf/Phoenix	Wool alcohol ointment DAB	30711310	1
Beiersdorf AG	Wool alcohol ointment DAB	30721310	1
Phönix	Wool alcohol ointment DAB	30821610	1
Beiersdorf/Gehe	Wool alcohol ointment DAB	30731210	1
Caelo	Wool alcohol ointment DAB	30831410	1
AHD, 05.04.2013	Wool alcohol ointment DAB	30831410	1
Phoenix	Wool alcohol ointment DAB	30831410	1
Beiersdorf/Phönix	Wool alcohol ointment DAB	30841410	1
Beiersdorf	Wool alcohol ointment DAB	30851510	1
Phönix Gotha	Wool alcohol ointment DAB	31231810	1
Caelo	Wool alcohol ointment DAB	31251910	1
Beiersdorf AG	Wool alcohol ointment DAB	31251910	1
Beiersdorf	Wool alcohol ointment DAB	31322010	1
Grokhhandel	Wool alcohol ointment DAB	31322010	1
Beiersdorf/ Noweda	Wool alcohol ointment DAB	31322010	1
Gehe	Wool alcohol ointment DAB	31322010	1
Phoenix	Wool alcohol ointment DAB	32344210	1
Anzag	Wool alcohol ointment DAB	3312E-01370	1
Beiersdorf AG	Wool alcohol ointment DAB	33323210	1
Beiersdorf / Noweda	Wool alcohol ointment DAB	33343310	1
BDF/ Noweda	Wool alcohol ointment DAB	33343310	1
Beiersdorf/Phoenix	Wool alcohol ointment DAB	33723610	1
eucerinum	Wool alcohol ointment DAB	33753710	1
Beiersdorf AG	Wool alcohol ointment DAB	34344210	1
eucerinum	Wool alcohol ointment DAB	34554710	1
Beiersdorf AG/Noweda	Wool alcohol ointment DAB	34414610	1
Defektur	Wool alcohol ointment DAB	3812	1
Defektur	Wool alcohol ointment DAB	40/13	1
Caelo	Wool alcohol ointment DAB	44/AKD9	1
Defektur	Wool alcohol ointment DAB	47/13	1
Phönix/beiersdorf	Wool alcohol ointment DAB	50955510	1
Defektur	Wool alcohol ointment DAB	53/13	1
Caelo	Wool alcohol ointment DAB	U-240513-3	1

- 52 480 spectra from 329 *Apo-Ident* customers from a total of 18 208 batches from a further 317 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 *Paraffin classification* 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 *Paraffin classification* 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	2369	0	31 975
Type B	0	3513	14	59 877
Type C	0	5839	122	52 439

The substance/substance group *Paraffin classification* 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 % (> 99.9688 %)	100.0000 % (> 99.7467 %)
Type B	100.0000 % (> 99.9711 %)	99.6031 % (> 99.5180 %)
Type C	100.0000 % (> 99.5973 %)	97.9534 % (> 97.9030 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30874	31702	3.17	19.34
30877	31358	4.78	25.16
30932	30932	0.00	17.62
30933	30933	0.00	16.26
31009	31941	3.24	27.32
31010	31941	4.63	28.27
31168	31446	3.23	21.61
31174	31174	0.00	27.68
31228	31228	0.00	31.04
31272	31272	0.00	30.89
31292	31446	3.56	21.84
31351	31351	0.00	17.91
31358	31358	0.00	25.42
31437	31916	2.21	26.73
31441	32017	8.15	31.97
31445	31610	3.96	27.73
31446	31446	0.00	21.06
31456	31456	0.00	34.40
31468	31916	3.89	26.47
31473	31473	0.00	25.14
31522	31522	0.00	30.14
31541	31736	9.20	28.60
31567	31909	8.53	35.56
31570	31570	0.00	19.55
31586	31736	9.61	27.65

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31587	31702	3.24	21.58
31590	31736	7.96	30.01
31601	32495	3.44	26.74
31602	31602	0.00	35.33
31610	31610	0.00	27.39
31611	31909	6.34	37.27
31612	31456	5.70	35.31
31702	31702	0.00	19.43
31736	31736	0.00	28.40
31740	31740	0.00	30.94
31744	31744	0.00	28.78
31807	31602	5.02	36.03
31812	31812	0.00	29.73
31816	31816	0.00	15.18
31909	31909	0.00	36.33
31910	31910	0.00	38.46
31916	31916	0.00	25.07
31917	31917	0.00	27.30
31920	31920	0.00	15.51
31921	31921	0.00	30.80
31940	31940	0.00	22.22
31941	31941	0.00	23.64
31949	31744	1.94	27.19
31954	31602	2.66	34.97
31999	31999	0.00	26.62
32017	32017	0.00	37.01
32279	32279	0.00	16.72
32495	32495	0.00	30.60
32517	32517	0.00	31.61
32704	32704	0.00	30.59
32900	32900	0.00	30.33
32946	31174	6.35	25.39
32947	31999	8.20	26.18

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Pasta Cordes®**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30633-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Pasta Cordes®

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Pasta Cordes®*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Ichthyol	Pasta Cordes®	12A008	30633	30	20121017
Ichthyol	Pasta Cordes®	13A056	31084	40	1406053
Ichthyol	Pasta Cordes®	13A056	31673	40	20130411

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 110 spectra of 3 reference samples from the substance/substance group *Pasta Cordes*[®]. These samples are listed above in the [calibration samples](#) section.
- 34 234 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 30 spectra of 2 reference samples from the substance/substance group *Pasta Cordes*[®].

Supplier	Substance	Batch	Sample ID	Spectra
Ichthyol	<i>Pasta Cordes</i> [®]	12A008	30633 [†]	10
Ichthyol	<i>Pasta Cordes</i> [®]	13A056	31673 [†]	20

- 63 564 spectra from a total of 1475 batches from further 439 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.

- 75 spectra from 29 *Apo-Ident* customers from 19 batches from the substance/substance group *Pasta Cordes*[®].

Supplier	Substance	Batch	Spectra
Ichthyol /Gehe	<i>Pasta Cordes</i> [®]	12A182	1
Ichthyol /Noweda	<i>Pasta Cordes</i> [®]	13A056	3
ichthyol/Gehe	<i>Pasta Cordes</i> [®]	12A182	2

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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
Ichthyol	Pasta Cordes [®]	13A056	1
Ichthyol-Gesellschaft	Pasta Cordes [®]	13A056	1
Ichthyol/Phoenix	Pasta Cordes [®]	13A056	3
Caelo	Pasta Cordes [®]	13A056	1
ichthyol/Gehe	Pasta Cordes [®]	13A098	3
Ichthyol	Pasta Cordes [®]	13A098	3
ichthyol/Gehe	Pasta Cordes [®]	13A146	1
Ichthyol/Phönix	Pasta Cordes [®]	14A025	2
Ichthyol/Phönix	Pasta Cordes [®]	14A124	1
Ichthyol/Gehe	Pasta Cordes [®]	14A124	1
Ichthyol	Pasta Cordes [®]	14A142	1
Ichthyol Gesellschaft C...	Pasta Cordes [®]	14A124	1
Fischer/Gehe	Pasta Cordes [®]	14A142	2
Ichthyol/Phönix	Pasta Cordes [®]	14A142	7
Ichthyol/Noweda	Pasta Cordes [®]	14A142	2
Ichthyol/ Phönix	Pasta Cordes [®]	14A142	1
Ichthyol / Noweda	Pasta Cordes [®]	14A142	1
Ichthyol Gesellschaft/K...	Pasta Cordes [®]	15A121	1
Phönix/Ichthyol	Pasta Cordes [®]	15A121	2
Ichthyol/Phoenix	Pasta Cordes [®]	15A121	1
Ichthyol Gesellschaft/N...	Pasta Cordes [®]	15A121	1
Ichthyol-Gesellschaft	Pasta Cordes [®]	15A121	1
Ichthyol/Phoenix	Pasta Cordes [®]	15A173	1
Ichthyol/Sanacorp	Pasta Cordes [®]	15A173	1
Ichthyol/Noweda	Pasta Cordes [®]	15A173	1
Ichthyol Cordes/Phoenix	Pasta Cordes [®]	15A173	1
Ichthyol Ges	Pasta Cordes [®]	11A069	1
Cordes / Phönix	Pasta Cordes [®]	15A173	1
Ichthyol/Phoenix	Pasta Cordes [®]	16A063	1
ICHTHYOL	Pasta Cordes [®]	10A187	1
Ichthyol/Gehe	Pasta Cordes [®]	11A206	2
Caelo	Pasta Cordes [®]	11A206	2
Ichthyol	Pasta Cordes [®]	12A008	1
Ichthyol/Gehe	Pasta Cordes [®]	12A043	3
Phoenix	Pasta Cordes [®]	12A043	1
Ichthyol	Pasta Cordes [®]	12a043	1
Ichthyol/Sanacorp	Pasta Cordes [®]	12A138	1
Ichthyol	Pasta Cordes [®]	12a182	2
Phönix	Pasta Cordes [®]	12A182	1
Ichthyol /Noweda	Pasta Cordes [®]	12A182	1
Ichthyol Ges	Pasta Cordes [®]	12A138	1
Ichthyol/Phoenix	Pasta Cordes [®]	12A182	1
Caelo	Pasta Cordes [®]	12A182	2
Ichthyol / Gehe	Pasta Cordes [®]	12A182	1
Cordes/AHD	Pasta Cordes [®]	13A056	1
Caelo	Pasta Cordes [®]	12AD43	1
ichthyol gesellschaft	Pasta Cordes [®]	13A098	1

- 58 366 spectra from 332 *Apo-Ident* customers from a total of 20 073 batches from a further 328 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 *Pasta 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 *Pasta 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	110	0	34 234
Type B	0	30	0	63 375
Type C	0	74	1	57 826

The substance/substance group *Pasta 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 % (> 99.9691 %)	100.0000 % (> 94.5455 %)
Type B	100.0000 % (> 99.9714 %)	100.0000 % (> 80.0000 %)
Type C	100.0000 % (> 99.5973 %)	98.6667 % (> 94.6667 %)

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.

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
30633	31084	6.02	34.53
31084	31084	0.00	34.57
31673	31084	6.86	34.54

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Perfume oil vanilla
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30665-2017-07-04
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:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 vani...	10293212	30665	40	20101020
Caelo	Perfume oil vani...	13393501	31191	40	1403100
Caelo	Perfume oil vani...	13393501	31400	40	20131205
Caelo	Perfume oil vani...	14284107	31786	40	20140924

Validation samples

A total of 156 379 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 *Perfume oil vanilla*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 32 spectra of 2 reference samples from the substance/substance group *Perfume oil vanilla*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Perfume oil vanilla	14284107	31786 [†]	20
Caelo	Perfume oil vanilla	15316308	not required	12

- 63 562 spectra from a total of 1475 batches from further 439 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 *Perfume oil vanilla*.
- 58 441 spectra from 332 *Apo-Ident* customers from a total of 20 092 batches from a further 329 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](#).

[†]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*.

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	160	0	34 184
Type B	0	32	0	63 562
Type C	0	0	0	58 441

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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 81.2500 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30665	31191	7.04	56.55
31191	31191	0.00	57.61
31400	31191	2.85	60.36
31786	31191	11.19	58.83

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Permethrin 25% solution**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31177-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Permethrin 25% solution

Special notes

When selecting the *Permethrin 25% solution* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Permethrin 25% solution*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Infectopharm	Permethrin 25% s...	S031301.1	31177	40	1405128
Infectopharm	Permethrin 25% s...	S061401.1	31563	40	1508108
Infectopharm	Permethrin 25% s...	S021601.1	32262	40	20160310
Infectopharm	Permethrin 25% s...	S021601.1	32263	40	20160310
Infectopharm	Permethrin 25% s...	S071602.1	33247	40	20160728

Validation samples

A total of 156 379 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 *Permethrin 25% solution*. These samples are listed above in the [calibration samples](#) section.
- 34 144 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 100 spectra of 3 reference samples from the substance/substance group *Permethrin 25% solution*.

Supplier	Substance	Batch	Sample ID	Spectra
Infectopharm	Permethrin 25% solution	S061101.1	30583	40
Infectopharm	Permethrin 25% solution	S021201.1	30584	40
Infectopharm	Permethrin 25% solution	S061401.1	31563 [†]	20

- 63 494 spectra from a total of 1474 batches from further 439 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.

- 117 spectra from 50 *Apo-Ident* customers from 41 batches from the substance/substance group *Permethrin 25% solution*.

Supplier	Substance	Batch	Spectra
InfectoPharm	Permethrin 25% solution	2091402	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
InfectoPharm	Permethrin 25% solution	5011501	1
InfectoPharm	Permethrin 25% solution	4071506	1
InfectoPharm	Permethrin 25% solution	9101406	1
Caelo	Permethrin 25% solution		4
InfectoPharm	Permethrin 25% solution	17121403	1
InfectoPharm	Permethrin 25% solution	11091403	1
InfectoPharm	Permethrin 25% solution	20081401	1
InfectoPharm	Permethrin 25% solution	14041401	1
infectopharm	Permethrin 25% solution	23071414	1
InfectoPharm	Permethrin 25% solution	31071402	1
InfectoPharm	Permethrin 25% solution	25111401	1
Phoenix	Permethrin 25% solution		3
InfectoPharm	Permethrin 25% solution	28011504	1
Infectopharm/Phoenix	Permethrin 25% solution		4
InfectoPharm	Permethrin 25% solution	S0216011	1
InfectoPharm	Permethrin 25% solution		7
Infectopharm	Permethrin 25% solution		17
Euro OTC	Permethrin 25% solution		1
Infectopharm	Permethrin 25% solution	S0614011	1
Noweda/InfectoPharm	Permethrin 25% solution		1
infectopharm	Permethrin 25% solution		1
Noweda/ Infectopharm	Permethrin 25% solution		1
Infectopharm/AHD	Permethrin 25% solution		6
Phoenix/InfectoPharm	Permethrin 25% solution		5
Infectopharm / 20	Permethrin 25% solution		1
InfectoPharm/Gehe	Permethrin 25% solution		2
Infectopharm/Ebert	Permethrin 25% solution		1
InfectoPharm/Phönix	Permethrin 25% solution		1
Infectopharm/Sanacorp	Permethrin 25% solution		2
Infectopharm/ Sanacorp	Permethrin 25% solution		3
InfectoPharma / Noweda	Permethrin 25% solution		1
Infectopharm / Noweda	Permethrin 25% solution		2
Infectopharm/Phönix	Permethrin 25% solution		3
Infectopharm/Sana	Permethrin 25% solution		1
Infectopharm/Noweda	Permethrin 25% solution		3
Phönix/Infectopharm	Permethrin 25% solution		1
InfectoPharm	Permethrin 25% solution	8011424	1
InfectoPharm	Permethrin 25% solution	6011407	1
Infectopharm	Permethrin 25% solution	S1214021	1
Anzag (Hersteller: Infe...	Permethrin 25% solution		1
InfectoPharm	Permethrin 25% solution	11061302	1
InfectoPharm	Permethrin 25% solution	2510210212011	1
InfectoPharm	Permethrin 25% solution	25021307	1
InfectoPharm	Permethrin 25% solution	21121202	1
InfectoPharm	Permethrin 25% solution	23111205	1
Infectopharm/ Phoenix	Permethrin 25% solution		1
Infectopharm, von Humbo...	Permethrin 25% solution		3
InfectoPharm/ G	Permethrin 25% solution		1
Infectopharm/ Now	Permethrin 25% solution		2
Infecto/Phönix	Permethrin 25% solution		1
infecto Pharma	Permethrin 25% solution		4
Infectopharm	Permethrin 25% solution	S0313011	1
Löwen City-Apotheke Bar...	Permethrin 25% solution		1
Noweda	Permethrin 25% solution		2
Gehe	Permethrin 25% solution		1
infectopharm/Jenne	Permethrin 25% solution		1
Infectopharm/ Noweda	Permethrin 25% solution		1
Infectopharm	Permethrin 25% solution	S081202	1
Infectopharm/Phönix	Permethrin 25% solution	S0313011	1
Infecto Pharm	Permethrin 25% solution		1

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Supplier	Substance	Batch	Spectra
infecto pharm	Permethrin 25% solution	s121402	1

- 58 324 spectra from 332 *Apo-Ident* customers from a total of 20 052 batches from a further 328 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 *Permethrin 25% solution* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Permethrin 25% solution* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive/negative*) and the validation spectrum type (*A/B/C*).

	False positive	True positive	False negative	True negative
Type A	0	200	0	34 144
Type B	0	100	0	63 494
Type C	0	103	14	58 324

The substance/substance group *Permethrin 25% solution* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate (specificity)* and the weighted *true positive rate (recognition rate)* are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9690 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.5964 %)	88.0342 % (> 85.4701 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31177	31177	0.00	99.92
31563	31563	0.00	135.08
32262	31563	7.08	122.39
32263	31563	4.59	125.17
33247	31177	8.45	97.14

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Peru balsam, original
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30862-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Peru balsam, original; Balsamum peruvianum verum

Special notes

When selecting the *Peru balsam, original* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Peru balsam, original*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Peru balsam, ori...	12302401	30862	40	20121017
Fagron	Peru balsam, ori...	13F13-N04	31293	40	1502255
Caelo	Peru balsam, ori...	14223909	31573	40	1703349

Validation samples

A total of 156 379 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 *Peru balsam, original*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 20 spectra of 1 reference samples from the substance/substance group *Peru balsam, original*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Peru balsam, original	14223909	31573 [†]	20

- 63 574 spectra from a total of 1476 batches from further 439 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 22 *Apo-Ident* customers from 17 batches from the substance/substance group *Peru balsam, original*.

Supplier	Substance	Batch	Spectra
Fagron	Peru balsam, original	12K30-N02	2
Fagron	Peru balsam, original	3913E-01162	1
Phönix Gotha	Peru balsam, original	10C30-N07	1
Fagron	Peru balsam, original	11G22-N06	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
Caelo	Peru balsam, original	11150808	3
Löwen City-Apotheke Bar...	Peru balsam, original	11G22-N06	1
Fagron	Peru balsam, original	9G03-N09	1
Caelo	Peru balsam, original	12020602	4
Caelo	Peru balsam, original	12020611	3
Fagron	Peru balsam, original	12302411	1
Caelo	Peru balsam, original	12302411	3
Fagron	Peru balsam, original	12A20-N13	1
Caelo	Peru balsam, original	12302413	1
Fagron	Peru balsam, original	2215I-01162	1
Caelo	Peru balsam, original	131966609	1
s.Prüfprotokoll	Peru balsam, original		1
Caelo	Peru balsam, original	13196606	2
Caelo	Peru balsam, original	Retest	1
Caelo	Peru balsam, original	13196609	1

- 58 411 spectra from 332 *Apo-Ident* customers from a total of 20 076 batches from a further 328 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 *Peru balsam, original* 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 *Peru balsam, original* 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	34 224
Type B	0	20	0	63 574
Type C	0	27	3	58 411

The substance/substance group *Peru balsam, original* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9712 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.5966 %)	90.0000 % (> 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.

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
30862	31293	17.92	101.86
31293	31293	0.00	108.14
31573	31573	0.00	124.93

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Petroleum ether
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30899-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Petroleum ether; Aether petrolei; Benzinum (petrolei)

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Petroleum ether*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Petroleum ether	12279604	30899	60	1503677
Otto Fischar	Petroleum ether	6323042	31253	40	1505436
Caelo	Petroleum ether	13141304	31283	40	1412255

Validation samples

A total of 156 379 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 *Petroleum ether*. These samples are listed above in the [calibration samples](#) section.
- 34 204 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Petroleum ether*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Petroleum ether	91883269	30102	40
Hedinger	Petroleum ether	28175B	32955	40

- 63 514 spectra from a total of 1475 batches from further 439 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.

- 829 spectra from 175 *Apo-Ident* customers from 187 batches from the substance/substance group *Petroleum ether*.

Supplier	Substance	Batch	Spectra
Hedinger/Gehe	Petroleum ether	28170B	2
Hedinger/AHD	Petroleum ether	28174B	1
Hedinger/Anzag	Petroleum ether	28171B	2
Hedinger	Petroleum ether	28171B	21
Hedinger	Petroleum ether	28172b	1
Hedinger/Phönix	Petroleum ether	28174B	2

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Supplier	Substance	Batch	Spectra
Hedinger	Petroleum ether	28174B	12
Hedinger/Phoenix	Petroleum ether	28175B	1
Fischar	Petroleum ether	6323097	1
Otto Fischar GmbH	Petroleum ether	6324063	1
Caelo	Petroleum ether	6326031	1
Hedinger	Petroleum ether	28169B	10
Fischar/Phoenix	Petroleum ether	6326047	1
Hedinger/AHD	Petroleum ether	28167B	2
Fischar/Spangro	Petroleum ether	6326026	1
Fischar/Gehe	Petroleum ether	6323093	1
Fischar GmbH	Petroleum ether	6323066	1
	Petroleum ether		1
Hedinger	Petroleum ether	2071202	1
Noweda	Petroleum ether	281658	1
Hedinger	Petroleum ether	28165B	6
Hedinger	Petroleum ether	281658	1
Hedinger/ Phönix	Petroleum ether	(028)028	1
Caelo	Petroleum ether	281668	3
Hedinger	Petroleum ether	28166B	9
Hedinger, Heiligenwiese...	Petroleum ether	28166B	2
Hedinger/Noweda	Petroleum ether	281678	1
Hedinger	Petroleum ether	281678	1
Noweda/Hedinger	Petroleum ether	28166B	1
Caelo	Petroleum ether	28166B	1
Hedinger/Otto	Petroleum ether	281678	1
Hedinger	Petroleum ether	28167B	17
Klenk	Petroleum ether	28167b	1
Hedinger / Gehe	Petroleum ether	28167B	1
Hedinger Phönix	Petroleum ether	28167B	1
Hedinger/Stumpf	Petroleum ether	28167B	1
Hedinger/Anzag 20.11.2012	Petroleum ether	28167B	2
Hedinger/Anzag	Petroleum ether	28167B	2
Hedinger/Gehe	Petroleum ether	28167B	2
heidinger/gehe	Petroleum ether	28167B	1
Hedinger	Petroleum ether	281688	2
Hedinger	Petroleum ether	28168B	17
Anzag/Hedinger	Petroleum ether	28167B	1
hedinger	Petroleum ether	28168B	1
Gehe/ Hedinger	Petroleum ether	28167B	1
hedinger/phönix	Petroleum ether	28167b	1
Hedinger/Gehe	Petroleum ether	28168B	2
Hedinger/ jenne	Petroleum ether	28168B	3
Caelo	Petroleum ether	28168B	3
Hedinger/Sanacorp	Petroleum ether	28168B	3
Hedinger/Phoenix	Petroleum ether	28168B	1
Noweda	Petroleum ether	281698	1
Caelo	Petroleum ether	281698	1
hedinger/noweda	Petroleum ether	281698	1
Hedinger	Petroleum ether	281698	2
hedinger/anzag	Petroleum ether	28169B	1
Hedinger/AHD	Petroleum ether	28169B	1
Hedinger / Gehe	Petroleum ether	28169B	3
Spangr/Hedinger	Petroleum ether	28169B	1
Caelo	Petroleum ether	28169B	5
Sanacorp	Petroleum ether	28169B	1
Hedinger	Petroleum ether	28170B	9
hedinger/noweda	Petroleum ether	28169B	1
Hedinger / Sanacorp	Petroleum ether	28169B	2
Hedinger , Stuttgart	Petroleum ether	28170B	1
Hedinger / Gehe	Petroleum ether	28170B	1

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Supplier	Substance	Batch	Spectra
Hedinger / NOW	Petroleum ether	28170B	1
Hedinger/Jenne	Petroleum ether	28170B	4
Hedinger/Sanacorp	Petroleum ether	28170B	1
Hedinger/V.d.L.	Petroleum ether	28170B	1
Barthel	Petroleum ether	28171B	3
HEDINGER / 20	Petroleum ether	28170B	1
Hedinger/Phönix	Petroleum ether	28171B	5
Hedinger/GEHE	Petroleum ether	28171B	1
Caelo	Petroleum ether	28171B	4
Hedinger / Gehe	Petroleum ether	28171B	1
hedinger/gehe	Petroleum ether	28171B	1
Spangro/Hedinger	Petroleum ether	28171B	1
Hedinger/Noweda	Petroleum ether	28171B	1
A. Hedinger / Noweda	Petroleum ether	281728	1
Hedinger	Petroleum ether	28172B	29
Caelo	Petroleum ether	28172B	2
Hedinger / Noweda	Petroleum ether	28172B	2
Hedinger/Sanacorp	Petroleum ether	28172b	1
Hedinger/Sanacorp	Petroleum ether	28172B	3
phoenix/hedinger	Petroleum ether	28172B	1
Hedinger/Gehe	Petroleum ether	28172B	1
Hedinger	Petroleum ether	28173B	13
Hedinger/Gehe	Petroleum ether	28173B	5
Caelo	Petroleum ether	28173B	1
Hedinger/AHD	Petroleum ether	28173B	1
Hedinger/Alliance Healt...	Petroleum ether	28174B	1
Hedinger Phönix	Petroleum ether	28174B	1
Hedinger/Noweda	Petroleum ether	28174B	4
Caelo	Petroleum ether	28174B	1
Hedinger/Sanacorp	Petroleum ether	28174B	1
Hedinger	Petroleum ether	28175B	2
Hedinger/Gehe	Petroleum ether	28174B	1
Calo/AHD	Petroleum ether	28175B	1
Caelo	Petroleum ether	28175B	3
Hedinger	Petroleum ether	3071304	1
Hedinger	Petroleum ether	3071401	1
Caelo	Petroleum ether	4031404	1
Caelo	Petroleum ether	11357104	1
Otto Fischer GmbH	Petroleum ether	15031402	1
Jenne	Petroleum ether	15045203	1
otto fischer	Petroleum ether	15081602	1
Hedinger/GEHE	Petroleum ether	1914M1170	1
Hedinger	Petroleum ether	2411Q-01170	1
Hedinger	Petroleum ether	25021302	1
Hedinger	Petroleum ether	28011506	1
Hedinger GmbH/Noweda	Petroleum ether	281738	1
Hedinger/ Noweda	Petroleum ether	281698	1
Fischar	Petroleum ether	24061501	1
Hedinger	Petroleum ether	29041501	1
Hedinger	Petroleum ether	31101203	1
Hedinger	Petroleum ether	30101310	1
Fischar / Phönix	Petroleum ether	3412I-01170	1
Fischar / Phönix	Petroleum ether	3413J-01170	1
Fischar	Petroleum ether	55780	1
Fischar	Petroleum ether	412062-2-P	1
Fischar/Gehe	Petroleum ether	3623111	1
Otto Fischar GmbH	Petroleum ether	6321091	1
fischar	Petroleum ether	6320031	1
Phönix	Petroleum ether	6321111	1
Fischar	Petroleum ether	6322041	1

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Supplier	Substance	Batch	Spectra
Phönix/Fischar	Petroleum ether	6322044	6
Fischar	Petroleum ether	6321111	1
Otto Fischar GmbH	Petroleum ether	6322045	1
Fischer Saarbrücken/GEHE	Petroleum ether	6322041	1
Fischar/Gehe	Petroleum ether	6322053	1
Fischar	Petroleum ether	6322061	1
Fischar	Petroleum ether	6322051	1
Gehe	Petroleum ether	6322061	1
Fischar	Petroleum ether	6322074	2
Fischar	Petroleum ether	632207A	2
Phoenix	Petroleum ether	6322074	1
Fischar	Petroleum ether	6322076	1
Fischar/Gehe	Petroleum ether	6322061	1
Fischar	Petroleum ether	6322079	1
Gehe	Petroleum ether	6322095	1
Fischar / Anzag	Petroleum ether	6322095	1
Phönix	Petroleum ether	6322101	9
Anzag/Fischar	Petroleum ether	6322098	1
Caelo	Petroleum ether	6322097	1
Phönix/Fischar	Petroleum ether	6322102	16
Phönix/Fischar	Petroleum ether	6322103	1
Phönix/Fischar	Petroleum ether	6322112	6
Fischer/Phoenix	Petroleum ether	6322104	1
Phönix/Fischar	Petroleum ether	6322113	5
Fischar / Noweda	Petroleum ether	6322112	1
Großhandel	Petroleum ether	6322113	1
Otto Fischar	Petroleum ether	6322116	1
Fischar	Petroleum ether	6322114	1
Fischar	Petroleum ether	6322113	1
Fischar/Gehe	Petroleum ether	6322117	1
gehe, 14.01.2013	Petroleum ether	6322117	1
Phönix	Petroleum ether	6322118	6
GEHE	Petroleum ether	6322119	1
Fischar	Petroleum ether	6322119	1
Phönix/ Fischar	Petroleum ether	6323015	12
Fagron	Petroleum ether	6323014	3
Fischar	Petroleum ether	6323017	1
Anzag/Fischar	Petroleum ether	6323017	1
Fischar	Petroleum ether	6323016	1
Fischar/Noweda	Petroleum ether	6323017	1
Fischar/Phoenix	Petroleum ether	6323016	1
Fischar	Petroleum ether	6323042	11
Großhandel	Petroleum ether	6323032	1
Fischar GmbH	Petroleum ether	6323022	1
Fischer Saarbrücken/GEHE	Petroleum ether	6323043	1
Fischar / Sanacorp	Petroleum ether	6323062	1
Fischar/Anzag	Petroleum ether	6323062	1
Fischar	Petroleum ether	6323063	3
Fischar/Phönix	Petroleum ether	6323063	1
Otto Fischar	Petroleum ether	6323063	1
Fischar/ Now	Petroleum ether	6323064	1
fischar/phoenix	Petroleum ether	6323064	1
Fischar/Noweda	Petroleum ether	6323065	1
Fischer	Petroleum ether	6323064	1
Fischar	Petroleum ether	6323067	6
Fischar	Petroleum ether	6323066	1
otto fischar/Sana	Petroleum ether	6323065	1
Caelo	Petroleum ether	6323068	17
Fischar	Petroleum ether	6323068	1
Fischar	Petroleum ether	6323091	6

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Supplier	Substance	Batch	Spectra
Fischar/Phoenix	Petroleum ether	6323069	1
Otto Fischar Phönix	Petroleum ether	6323069	1
Fischar/Noweda	Petroleum ether	6323069	1
Ebert/Fischar	Petroleum ether	6323093	1
Fischar / Noweda	Petroleum ether	6323069	1
Fischar	Petroleum ether	6323093	7
Fischar/Anzag	Petroleum ether	6323095	1
FISCHER GMBH / GEHE	Petroleum ether	6323094	1
Fischer/Sanacorp	Petroleum ether	6323099	1
Fischar/Anzag	Petroleum ether	6323099	1
Otto Fischar GmbH	Petroleum ether	6323094	1
Fischar	Petroleum ether	6323099	1
Otto Fischar Phönix	Petroleum ether	6323111	1
Großhandel	Petroleum ether	6323111	1
Fischar	Petroleum ether	6323112	5
Fischar	Petroleum ether	6324013	1
Fischar/Gehe	Petroleum ether	6323113	1
Fischar	Petroleum ether	6324016	1
Fischar/Nowenda	Petroleum ether	6323112	1
Caelo	Petroleum ether	6324017	29
Caelo	Petroleum ether	6324018	5
Alliance Healthcare/Fis...	Petroleum ether	6324025	1
Fischar	Petroleum ether	632401A	1
Fischar Phönix	Petroleum ether	6324018	1
Fischar/Phoenix	Petroleum ether	6324018	1
Fischar/Sanacorp	Petroleum ether	6324033	1
Fischar/ Phönix	Petroleum ether	6324034	13
Fischar	Petroleum ether	6324034	2
Phoenix/Fischar	Petroleum ether	6324035	5
Otto Fischar/Gehe	Petroleum ether	6324035	1
Fischar	Petroleum ether	6324041	2
fishar	Petroleum ether	6324035	1
Phönix/Fischar	Petroleum ether	6324051	28
Caelo	Petroleum ether	6324042	1
Fischer	Petroleum ether	6324062	1
Fischar/Anzag	Petroleum ether	6324063	1
Fischar	Petroleum ether	6324064	8
Fischar/Alliance Heathc...	Petroleum ether	6324064	1
Fischar/Sanacorp	Petroleum ether	6324065	1
Fischar	Petroleum ether	6324072	14
Fischar	Petroleum ether	6324074	1
Noweda / Fischer	Petroleum ether	6324075	1
Fischar	Petroleum ether	6324082	15
Caelo	Petroleum ether	6324082	2
Fischar	Petroleum ether	6324075	1
Fischer	Petroleum ether	6324095	1
Fischer	Petroleum ether	6324102	1
Fischbar	Petroleum ether	6324103	1
FISCHER GMBH / GEHE	Petroleum ether	6324091	1
Fischar	Petroleum ether	6324104	3
Fischar/Phönix	Petroleum ether	6324105	1
Fischar / Phoenix	Petroleum ether	6324093	1
Fischar	Petroleum ether	6324083	1
Fischar	Petroleum ether	6324105	4
Caelo	Petroleum ether	6324113	1
Fagron	Petroleum ether	6324114	1
Fischar	Petroleum ether	6324114	2
Fiebig	Petroleum ether	6324123	1
Caelo	Petroleum ether	6325021	1
Fischar/Phönix	Petroleum ether	6324123	1

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Supplier	Substance	Batch	Spectra
Fischar	Petroleum ether	6325022	2
Caelo	Petroleum ether	6325034	3
Fischer/Phönix	Petroleum ether	6325014	1
Fischar	Petroleum ether	6325012	1
Fischar	Petroleum ether	6325025	1
Fischar	Petroleum ether	6325024	1
Fischar GmbH	Petroleum ether	6325044	1
Fischar	Petroleum ether	6325042	1
Fischar	Petroleum ether	6325051	1
Fischar/Phoenix	Petroleum ether	6325051	1
Fischar	Petroleum ether	6325052	1
Otto Fischer/Sanacorp	Petroleum ether	6325051	1
Fischar/Anzag	Petroleum ether	6325053	1
Caelo	Petroleum ether	6325055	2
Fischar	Petroleum ether	6325063	3
Otto Fischer	Petroleum ether	6325063	1
Fischer/Phönix	Petroleum ether	6325081	3
Otto Fischer / Sanacorp	Petroleum ether	6325083	1
Fischar/Alliance H.	Petroleum ether	6325104	1
Fischer/Sanacorp	Petroleum ether	6325105	1
Fischer	Petroleum ether	6325107	1
Fischar/ Sanacorp	Petroleum ether	6325108	1
Sanacorp	Petroleum ether	632510A	1
Fischar	Petroleum ether	6325109	1
Caelo	Petroleum ether	6325111	2
Fischar/Noweda	Petroleum ether	6326011	1
Fischar	Petroleum ether	6326011	1
Otto Fischer/Phönix	Petroleum ether	6326026	4
fischar	Petroleum ether	6326021	2
Caelo	Petroleum ether	6326014	1
Fischar	Petroleum ether	6326012	1
Otto Fischer/Noweda	Petroleum ether	6325119	1
Otto Fischer GmbH & Co...	Petroleum ether	6325111	1
fischar/Sanacorp	Petroleum ether	6326026	1
Fischar/Alliance Health...	Petroleum ether	6326027	2
Otto Fischer/Gehe	Petroleum ether	6326027	1
Otto Fischer	Petroleum ether	6326052	1
Fischar/Sanacorp	Petroleum ether	6326047	1
Otto Fischer/Phönix	Petroleum ether	6326047	1
Fischar/phoenix	Petroleum ether	6326061	5
Caelo	Petroleum ether	6326063	1
Otto Fischer GmbH & Co...	Petroleum ether	X81A41	1
Hedinger/Otto	Petroleum ether		1
Phoenix	Petroleum ether	6326072	1
Noweda	Petroleum ether	28164B	1
Gehe	Petroleum ether	28166B	1
Hedinger/N/08.05.13/PZN...	Petroleum ether	28167B	1
Fischar Phönix	Petroleum ether	6323094	1
Stumpf/Hedinger	Petroleum ether	281718	1
Hedinger/Phönix	Petroleum ether	28167B	2
Hedinger/Phönix	Petroleum ether	28172B	1
Fischar Phönix	Petroleum ether	6323112	1
Anzag/Hedinger	Petroleum ether	28172B	1
Phoenix/hedinger	Petroleum ether	28169B	2
Phoenix/hedinger	Petroleum ether	28168B	1
Fischar	Petroleum ether	7283797	1
Fischar	Petroleum ether	6323033	1
Fischar	Petroleum ether	6322073	1
Hedinger/Sanacorp	Petroleum ether	28169B	4
Hedinger	Petroleum ether	204311170	1

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Supplier	Substance	Batch	Spectra
Hedinger/Noweda	Petroleum ether	21728	1
Hedinger / Anzag	Petroleum ether	28163B	1
Hedinger/Anzag 11.06.2012	Petroleum ether	28166B	1
Anzag 21.08.2012	Petroleum ether	28166b	1
Hedinger, Noweda	Petroleum ether	28166B	2
Noweda	Petroleum ether	28166B	1
Hedinger/Sanacorp	Petroleum ether	28166B	1
Hedinger, Noweda	Petroleum ether	28167B	3
Caelo	Petroleum ether	28167B	1
Kruger/Hedinger/06.01.14	Petroleum ether	28167B	1
anzag 15.11.12	Petroleum ether	28167B	1
Hedinger/Stumpf	Petroleum ether	28168B	1
Phönix	Petroleum ether	28168B	1
Hedinger, Noweda	Petroleum ether	28168B	2
Noweda/Hedinger	Petroleum ether	28168B	2
HEDINGER / 20	Petroleum ether	28168B	1
Hedinger / Anzag	Petroleum ether	28168B	1
Hedinger/Otto	Petroleum ether	281698	1
Hedinger/Sanacorp	Petroleum ether	281698	1
Hedinger/Phönix	Petroleum ether	28169B	3
Phönix	Petroleum ether	28169B	1
Stumpf / Hedinger	Petroleum ether	28169B	1
Noweda	Petroleum ether	28169B	1
Hedinger / Noweda	Petroleum ether	28169B	1
Dr. Seeger/ Phönix	Petroleum ether	28169B	1
Caelo	Petroleum ether	28170B	1
A.Hedinger / Kehr	Petroleum ether	281708	1
Noweda/Hedinger	Petroleum ether	28170B	1
Hedinger/Holdermann	Petroleum ether	28170B	1
Hedinger/V.d.L.	Petroleum ether	28171B	1
Sanacorp	Petroleum ether	28171B	1
Jenne	Petroleum ether	28171B	2
Phoenix	Petroleum ether	28171B	1
HEDINGER / 30	Petroleum ether	28172B	2
Stumpf/Hedinger	Petroleum ether	28172B	1
Hedinger / Phoenix	Petroleum ether	28172B	1
Hedinger/Noweda	Petroleum ether	28173B	2
Jenne	Petroleum ether	28173B	1
Hedinger/ Sanacorp	Petroleum ether	28173B	1
Hedinger über Sanacorp	Petroleum ether	28173B	1
Heidinger/Anzag	Petroleum ether	28174B	1
Hedinger/Anzag	Petroleum ether	28174B	1
Noweda/Hedinger	Petroleum ether	28174B	1
Euro OTC	Petroleum ether	28174B	1
Hedinger	Petroleum ether	12121401	1
Caelo	Petroleum ether	13141302	1
Hedinger, Heiligenwiese...	Petroleum ether		1
Hedinger	Petroleum ether	13081309	1
Hedinger	Petroleum ether	15091402	1
Kost/kost	Petroleum ether	4065061213	1
Euro OTC	Petroleum ether	2304123	1
Fischar/Anzag	Petroleum ether	6323016	1
Fischar	Petroleum ether	6323032	8
Fischar/Anzag	Petroleum ether	6323024	1
Fischar/ Phönix	Petroleum ether	6323081	12
Fischar/Gehe	Petroleum ether	6324062	1
Anzag/Fischar	Petroleum ether	6324064	1
Fischar/ Noweda	Petroleum ether	6324104	1
Fischar/ Phönix	Petroleum ether	6325106	1
Caelo	Petroleum ether	64/AKD53	1

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Supplier	Substance	Batch	Spectra
Großhandel	Petroleum ether		1
otto fischer/Phoenix	Petroleum ether	6325044	1
Alliance/ Hedinger	Petroleum ether	Y50L63	1
Sanacorp	Petroleum ether		1

- 57 612 spectra from 332 *Apo-Ident* customers from a total of 19 909 batches from a further 328 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 *Petroleum ether* 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 *Petroleum ether* 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	34 204
Type B	0	80	0	63 514
Type C	0	811	18	57 612

The substance/substance group *Petroleum ether* 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 % (> 99.9690 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5963 %)	97.8287 % (> 97.4668 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30899	30899	0.00	30.69
31253	31253	0.00	35.52
31283	31283	0.00	30.28

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Petroleum oil, white, cohobated
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31212-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Petroleum oil, white, cohobated; Oleum petrae album rectific.; Petroleum album rectific.

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Petroleum oil, white, cohobated*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Petroleum oil, w...	13146704	31212	40	1403110
Caelo	Petroleum oil, w...	14019607	31387	40	20140124

Validation samples

A total of 156 379 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 *Petroleum oil, white, cohobated*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 100 spectra of 3 reference samples from the substance/substance group *Petroleum oil, white, cohobated*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Petroleum oil, white, cohoba...	10356508	30411	40
Caelo	Petroleum oil, white, cohoba...	14019607	31387 [†]	20
Caelo	Petroleum oil, white, cohoba...	163278	33109	40

- 63 494 spectra from a total of 1474 batches from further 439 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 8 *Apo-Ident* customers from 12 batches from the substance/substance group *Petroleum oil, white, cohobated*.

Supplier	Substance	Batch	Spectra
Caelo	Petroleum oil, white, cohoba...	13086401	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
Caelo	Petroleum oil, white, cohoba...	14242201	1
Caelo	Petroleum oil, white, cohoba...	12173101	2
Caelo	Petroleum oil, white, cohoba...	13086402	1
Caelo	Petroleum oil, white, cohoba...	13303603	2
Caelo	Petroleum oil, white, cohoba...	13146702	3
Caelo	Petroleum oil, white, cohoba...	11379102	1
Caelo	Petroleum oil, white, cohoba...	11198403	1
Caelo	Petroleum oil, white, cohoba...	14019602	1
Caelo	Petroleum oil, white, cohoba...	14130105	1
Caelo	Petroleum oil, white, cohoba...	15035705	1
Caelo	Petroleum oil, white, cohoba...	12173103	1

- 58 425 spectra from 332 *Apo-Ident* customers from a total of 20 080 batches from a further 328 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 *Petroleum oil, white, cohobated* 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 *Petroleum oil, white, cohobated* 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	34 264
Type B	0	100	0	63 494
Type C	0	13	3	58 425

The substance/substance group *Petroleum oil, white, cohobated* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.5968 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31212	31212	0.00	33.55
31387	31212	4.49	33.25

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Phenoxyethanol**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31808-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Phenoxyethanol

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Phenoxyethanol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor	Phenoxyethanol	APDEG4324219P	31808	40	AR-16-FG-003720-01
Audor	Phenoxyethanol	APDEG4324219P	31953	40	20150219

Validation samples

A total of 156 379 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 *Phenoxyethanol*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 797 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 51 spectra of 2 reference samples from the substance/substance group *Phenoxyethanol*.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Phenoxyethanol	APDEG4324219P	31808 [†]	31
Audor Pharma	Phenoxyethanol	APDEG4324219P	31953 [†]	20

- 63 543 spectra from a total of 1476 batches from further 439 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 *Phenoxyethanol*.
- 58 441 spectra from 332 *Apo-Ident* customers from a total of 20 092 batches from a further 329 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](#).

[†]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*.

Validation results

The validation runs checked whether the substance/substance group *Phenoxyethanol* 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 *Phenoxyethanol* 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	34 264
Type B	0	51	0	63 543
Type C	0	0	0	58 441

The substance/substance group *Phenoxyethanol* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 88.2353 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31808	31808	0.00	52.86
31953	31808	3.92	52.77

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Phytomenadione**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30747-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Phytomenadione; Phytomenadionum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Phytomenadione*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Phytomenadione	12H31-N02	30747	40	1405178
Fagron	Phytomenadione	14I02-B04-301537	31621	40	20141210

Validation samples

A total of 156379 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 *Phytomenadione*. These samples are listed above in the [calibration samples](#) section.
- 34264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 20 spectra of 1 reference samples from the substance/substance group *Phytomenadione*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Phytomenadione	14I02-B04-301537	31621 [†]	20

- 63574 spectra from a total of 1476 batches from further 439 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 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Phytomenadione*.

Supplier	Substance	Batch	Spectra
Merck	Phytomenadione	EH14000190	1
Fagron	Phytomenadione	13D26-B07-286714	1
Merck	Phytomenadione	EH13000590	1
Fagron	Phytomenadione	13C25-N07	1

[†]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*.

- 58 437 spectra from 332 *Apo-Ident* customers from a total of 20 088 batches from a further 328 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 *Phytomenadione* 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 *Phytomenadione* 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	34 264
Type B	0	20	0	63 574
Type C	0	4	0	58 437

The substance/substance group *Phytomenadione* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9712 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.5985 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30747	30747	0.00	109.70
31621	30747	5.27	112.46

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Pine needle oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31183-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Pine needle oil; Oleum pini silvestris

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Pine needle oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Pine needle oil	13E24-N05	31183	40	1403166
Caelo	Pine needle oil	13334502	31202	40	1403168
Caelo	Pine needle oil	13334501	31405	40	20131009

Validation samples

A total of 156 379 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 *Pine needle oil*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Pine needle oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pine needle oil	10084705	30252	40
Caelo	Pine needle oil	16298401	33250	40

- 63 514 spectra from a total of 1475 batches from further 439 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 23 *Apo-Ident* customers from 25 batches from the substance/substance group *Pine needle oil*.

Supplier	Substance	Batch	Spectra
noweda	Pine needle oil	13334501	2
Phönix	Pine needle oil	13334501	2
Caelo	Pine needle oil	13334501	4
Fagron	Pine needle oil	14J27-B06	1
Caelo	Pine needle oil	15239101	2
Fagron	Pine needle oil	15F12-B02-308878	1

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Supplier	Substance	Batch	Spectra
Taoasis	Pine needle oil	20017-118846	1
Caelo	Pine needle oil	26091404	1
Taoasis	Pine needle oil	28663-119531	1
Taoasis	Pine needle oil	28663-119029	1
Taoasis	Pine needle oil	28663-120876	2
Taoasis	Pine needle oil	35808-123038	2
Taoasis	Pine needle oil	8169-117244	4
Taoasis	Pine needle oil	49977-125240	1
Caelo	Pine needle oil	11024602	1
Caelo	Pine needle oil	11024603	1
Noweda	Pine needle oil	11161605	1
Caelo	Pine needle oil	12080504	4
Caelo	Pine needle oil	11161605	2
Caelo	Pine needle oil	12246905	1
Caelo	Pine needle oil	12246907	2
Caelo	Pine needle oil	122466904	1
Fagron	Pine needle oil	13E24-N05	1
Fagron	Pine needle oil	12G20-N04	1
Taoasis/Phönix	Pine needle oil	32372-110382	1
Taoasis	Pine needle oil	33717-112501	2
Taoasis	Pine needle oil	30600-18490	1
Fagron	Pine needle oil	12L03-N05	1

- 58 396 spectra from 332 *Apo-Ident* customers from a total of 20 067 batches from a further 328 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 *Pine needle 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 *Pine needle 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	34 224
Type B	0	70	10	63 514
Type C	0	41	4	58 396

The substance/substance group *Pine needle 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	87.5000 % (> 83.7500 %)
Type C	100.0000 % (> 99.5965 %)	91.1111 % (> 84.4444 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31183	31183	0.00	21.41
31202	31202	0.00	21.99
31405	31202	2.46	21.83

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Pine tar**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31221-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Pine tar; Pix liquida

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Pine tar*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pine tar	13008302	31221	40	1403320
Caelo	Pine tar	13008309	31614	40	20130116

Validation samples

A total of 156 379 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 *Pine tar*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Pine tar*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pine tar	73260048	30280	40
Caelo	Pine tar	13008309	31614 [†]	20

- 63 534 spectra from a total of 1475 batches from further 439 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 *Pine tar*.
- 58 441 spectra from 332 *Apo-Ident* customers from a total of 20 092 batches from a further 329 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](#).

[†]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*.

Validation results

The validation runs checked whether the substance/substance group *Pine tar* 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 *Pine tar* 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	34 264
Type B	0	20	40	63 534
Type C	0	0	0	58 441

The substance/substance group *Pine tar* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	33.3333 % (> 28.3333 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31221	31221	0.00	106.33
31614	31221	8.05	106.77

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Polyhexanide solution 20%
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30596-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Polyhexanide solution 20%; Polihexanidi solutio 20%; Solutio polyhexanidi 20%

Special notes

When selecting the *Polyhexanide solution 20%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Polyhexanide solution 20%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Polyhexanide sol. ...	13H05-N04	31180	40	1403256
Fagron	Polyhexanide sol. ...	13K29-B30-288935	31571	40	20131217
Fagron	Polyhexanide sol. ...	16B16-B04-322720	32733	40	20160229

Validation samples

A total of 156379 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 *Polyhexanide solution 20%*. These samples are listed above in the [calibration samples](#) section.
- 34224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 100 spectra of 3 reference samples from the substance/substance group *Polyhexanide solution 20%*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Polyhexanide solution 20%	12A04-N06	30596	40
Fagron	Polyhexanide solution 20%	13K29-B30-288935	31571 [†]	20
Fagron	Polyhexanide solution 20%	15H28-B11-313603	32276	40

- 63494 spectra from a total of 1474 batches from further 439 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.

- 131 spectra from 69 *Apo-Ident* customers from 44 batches from the substance/substance group *Polyhexanide solution 20%*.

Supplier	Substance	Batch	Spectra
Fargom	Polyhexanide solution 20%	116B16-B04-320854	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
Caelo	Polyhexanide solution 20%	13351M28	2
Fagron	Polyhexanide solution 20%	13H05-N04	9
GEHE 14.04.2014	Polyhexanide solution 20%	13K29-B30288934	1
Fagron	Polyhexanide solution 20%	13K29-B30	1
Fagron	Polyhexanide solution 20%	13K29-B30-288934	5
Caelo	Polyhexanide solution 20%	13K29-B30-288934	1
Caelo	Polyhexanide solution 20%	13K29-B30-288938	4
Fagron	Polyhexanide solution 20%	13K29-B30-288938	4
Fagron	Polyhexanide solution 20%	14F25-B06	8
Sanacorp	Polyhexanide solution 20%	14f25-b06-2962291	1
Fagron	Polyhexanide solution 20%	14F25-B06-296291	2
Caelo	Polyhexanide solution 20%	14F25-B06-296291	2
Caelo	Polyhexanide solution 20%	14F25-B06-296292	2
Fagron	Polyhexanide solution 20%	14F25-B06-296292	9
Gehe 16.12.14	Polyhexanide solution 20%	14F25-B06-296292	1
Fagron	Polyhexanide solution 20%	14F25-b06-296292	1
Fragon/Phönix	Polyhexanide solution 20%	14F25-B06-300092	1
Fagron	Polyhexanide solution 20%	14F25-B06-300092	3
Fagron	Polyhexanide solution 20%	14F25-B06-300093	4
Caelo	Polyhexanide solution 20%	14F25-B06-300093	2
Caelo	Polyhexanide solution 20%	14GR132285	1
Fagron	Polyhexanide solution 20%	14F25-B06-305013	2
Fagron	Polyhexanide solution 20%	14GR132285	1
Fagron	Polyhexanide solution 20%	14GR274618	1
Fagron	Polyhexanide solution 20%	15C20-B06-309678	3
Fagron	Polyhexanide solution 20%	15H28-B11	4
Noweda	Polyhexanide solution 20%	15H28-B11-312309	1
Fagron	Polyhexanide solution 20%	15H28-B11-313603	4
Fagron	Polyhexanide solution 20%	15H28-B11-312309	2
Euro OTC	Polyhexanide solution 20%	15H28-B11-313604	1
Fagron	Polyhexanide solution 20%	15H28-B11-315703	2
Fagron	Polyhexanide solution 20%	15H28-B11-313604	1
Fagron	Polyhexanide solution 20%	16B16-B04-320854	1
Fagron	Polyhexanide solution 20%	16B16-B04	3
Fagron	Polyhexanide solution 20%	16B16-B04-318789	1
Phoenix	Polyhexanide solution 20%	16B16-B04	1
Fagron	Polyhexanide solution 20%	16B16-B04-325487	2
Fragon GmbH	Polyhexanide solution 20%	16GR025056	1
Fagron	Polyhexanide solution 20%	18071501	1
Fagron	Polyhexanide solution 20%	2215I-03580	1
Fagron	Polyhexanide solution 20%	11GR180545	2
Fagron	Polyhexanide solution 20%	3714M-03580	1
Caelo	Polyhexanide solution 20%	12GR227646	1
Fagron	Polyhexanide solution 20%	12A04-N06	2
Caelo	Polyhexanide solution 20%	12B09-N01	1
Fagron	Polyhexanide solution 20%	12K20-N01	4
Fragon	Polyhexanide solution 20%	12K20-N01	1
Fagron	Polyhexanide solution 20%	12k20-n01	2
Noweda	Polyhexanide solution 20%	12K20-N01	1
Gehe 16.04.2013	Polyhexanide solution 20%	12K20-N01	1
Caelo	Polyhexanide solution 20%	12K20N01	1
Phoenix	Polyhexanide solution 20%	12K20-N01	1
B.Braun / Gehe	Polyhexanide solution 20%	13103M18	3
Fagron	Polyhexanide solution 20%	13H05-N01	7
Phytocomm	Polyhexanide solution 20%	27803278	1
Fagron	Polyhexanide solution 20%	13H05-No4	1
Ichthyol Gesellschaft/AHD	Polyhexanide solution 20%	14F25-B06-296292	1
Caelo	Polyhexanide solution 20%	14F25-B06	1
Fagron	Polyhexanide solution 20%	12D27-N07	1

- 58 310 spectra from 332 *Apo-Ident* customers from a total of 20 048 batches from a further 328 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 *Polyhexanide solution 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 *Polyhexanide solution 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	120	0	34 224
Type B	0	100	0	63 494
Type C	0	112	19	58 310

The substance/substance group *Polyhexanide solution 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.5964 %)	85.4962 % (> 83.2061 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31180	31180	0.00	27.75
31571	31180	8.20	28.27
32733	31180	12.00	30.59

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Polyol fatty acid ester
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30755-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Polyol fatty acid ester; Cetiol® HE

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Polyol fatty acid ester*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Polyol fatty aci...	11162809	30755	40	20110616
Caelo	Polyol fatty aci...	13292302	31179	40	1402589
Caelo	Polyol fatty aci...	13357702	31366	40	20131112

Validation samples

A total of 156 379 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 *Polyol fatty acid ester*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Polyol fatty acid ester*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Polyol fatty acid ester	pending	30567	40
Caelo	Polyol fatty acid ester	161120	32196	40

- 63 514 spectra from a total of 1476 batches from further 439 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.

- 44 spectra from 32 *Apo-Ident* customers from 17 batches from the substance/substance group *Polyol fatty acid ester*.

Supplier	Substance	Batch	Spectra
Caelo	Polyol fatty acid ester	13357703	2
Phönix	Polyol fatty acid ester	14033502	1
Caelo	Polyol fatty acid ester	14033502	4
Caelo	Polyol fatty acid ester	143033502	1
Caelo	Polyol fatty acid ester	15298004	1
Caelo	Polyol fatty acid ester		1

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Supplier	Substance	Batch	Spectra
Caelo	Polyol fatty acid ester	11081403	1
Caelo	Polyol fatty acid ester	11162809	1
GEHE	Polyol fatty acid ester	12361804	2
Caelo	Polyol fatty acid ester	11162811	1
Caelo	Polyol fatty acid ester	12361804	4
Caelo	Polyol fatty acid ester	12361808	4
Caelo	Polyol fatty acid ester	13158902	5
Caelo	Polyol fatty acid ester	13158901	1
Noweda	Polyol fatty acid ester	13158903	1
Caelo	Polyol fatty acid ester	13158903	4
Caelo	Polyol fatty acid ester	13158904	1
Caelo	Polyol fatty acid ester	13292302	4
Phönix	Polyol fatty acid ester	13357702	1
Caelo	Polyol fatty acid ester	13357702	3
Caelo	Polyol fatty acid ester	14322405	1

- 58 397 spectra from 332 *Apo-Ident* customers from a total of 20 075 batches from a further 328 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 *Polyol fatty acid ester* 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 *Polyol fatty acid ester* 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	34 224
Type B	0	80	0	63 514
Type C	0	44	0	58 397

The substance/substance group *Polyol fatty acid ester* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5965 %)	100.0000 % (> 86.3636 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30755	31179	8.22	17.36
31179	31179	0.00	18.84
31366	31179	5.96	18.90

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Polysorbate 80 / Macrogolglycerolricinoleat**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30766-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Polysorbate 80 / Macrogolglycerolricinoleat; Macrogolglycerol ricinoleate; Macrogolglyceroli ricinoleas; Poloxyaethylenglycerinum triricinoleinicum 35; Polysorbate 80; Polysorbatum 80

Special notes

When selecting the *Polysorbate 80 / Macrogolglycerolricinoleat* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Polysorbate 80 / Macrogolglycerolricinoleat*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Macrogolglycerol...	12E29-N02	30766	60	20120612
Caelo	Polysorbate 80	12116009	30893	80	20120427
Fagron	Macrogolglycerol...	12H08-N01	31015	40	20120827
Caelo	Polysorbate 80	13372015	31325	40	AR-15-FG-008176-01
Caelo	Macrogolglycerol...	13272708	31368	40	1505503

Validation samples

A total of 156 379 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 *Polysorbate 80 / Macroglycerolricinoleat*. These samples are listed above in the [calibration samples](#) section.
- 34 084 spectra from a total of 793 batches from further 223 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 130 spectra of 4 reference samples from the substance/substance group *Polysorbate 80 / Macroglycerolricinoleat*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Polysorbate 80	11179606	30395	40
Caelo	Polysorbate 80	12116009	30893 [†]	10
Caelo	Macroglycerol ricinoleate	161303	32297	40
Caelo	Macroglycerol ricinoleate	161545	32338	40

- 63 464 spectra from a total of 1473 batches from further 438 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.

- 208 spectra from 94 *Apo-Ident* customers from 74 batches from the substance/substance group *Polysorbate 80 / Macroglycerolricinoleat*.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Macrogolglycerol ricinoleate	15312304	1
Caelo	Macrogolglycerol ricinoleate	15312307	1
Fagron	Macrogolglycerol ricinoleate	13B08-N03	2
BASF Chem trade GmbH/Ph...	Macrogolglycerol ricinoleate	13B08-N03	1
Fagron	Macrogolglycerol ricinoleate	44242575L0	1
Fagron	Macrogolglycerol ricinoleate	13J24-B03-287433	1
Fagron	Macrogolglycerol ricinoleate	13E13-N11	2
Fagron	Macrogolglycerol ricinoleate	12G02-N11	1
Fagron	Macrogolglycerol ricinoleate	14L08-B04-302328	1
Fagron	Macrogolglycerol ricinoleate	13B08-No3	1
Fagron	Polysorbate 80	813I-02527	1
Caelo	Polysorbate 80	12315328	12
Caelo	Polysorbate 80	12315317	9
Caelo	Polysorbate 80	515I-02527	1
Caelo	Polysorbate 80	12315324	1
Caelo	Polysorbate 80	13152216	12
Caelo	Polysorbate 80	13152223	9
Caelo	Polysorbate 80	13152218	1
Nachprüfung 3008	Polysorbate 80	13152223	1
Caelo	Polysorbate 80	13372012	9
Caelo	Polysorbate 80	13372015	1
Gehe 01.07.2014	Polysorbate 80	13372015	1
Caelo	Polysorbate 80	1419026	1
Caelo	Polysorbate 80	14190306	2
Caelo	Polysorbate 80	14190316	13
ICHTHYOL/ahp	Polysorbate 80	14190310	1
Caelo	Polysorbate 80	14190317	1
Fagron	Polysorbate 80	14C24-B07	1
Fagron	Polysorbate 80	14C24-B07-296371	3
Fagron	Polysorbate 80	14K27-B01-307106	2
Fargon/Kehr	Polysorbate 80	14K27-B01-307106	1
Devesa/ Phönix	Polysorbate 80	14K27-Bo1-307106	1
Caelo	Polysorbate 80	15104103	7
Caelo	Polysorbate 80	15104112	9
Caelo	Polysorbate 80	15104121	2
Ebert u. Jacobi 24.06...	Polysorbate 80	15104112	1
Caelo	Polysorbate 80	15121404	1
Caelo	Polysorbate 80	15104113	1
Caelo	Polysorbate 80	15104126	3
Caelo	Polysorbate 80	16059402	6
Caelo	Polysorbate 80	16053402	1
Cealo/AHD	Polysorbate 80	16059402	1
GEHE	Polysorbate 80	16B17-B09	1
Caelo	Polysorbate 80	16260201	1
Caelo	Polysorbate 80	18081502	1
Caelo	Polysorbate 80	42175394	2
Fagron	Polysorbate 80	908ND3714	2
Fagron	Polysorbate 80	808ND3713	1
Fargon	Polysorbate 80	10114N07	1
Caelo	Polysorbate 80	10235202	1
Bombastus	Polysorbate 80	11347907	1
Caelo	Polysorbate 80	11179606	1
Caelo	Polysorbate 80	11347907	2
Caelo	Polysorbate 80	11179618	1
Fagron	Polysorbate 80	11L22-N12	1
Caelo	Polysorbate 80	12116005	4
Phoenix	Polysorbate 80	12116005	1
Caelo	Polysorbate 80	11347909	1
Caelo	Polysorbate 80	12116009	8
Caelo	Polysorbate 80	12116013	7

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continued from previous page

Supplier	Substance	Batch	Spectra
Phönix 04.07.2013	Polysorbate 80	12116013	1
Caelo	Polysorbate 80	12315308	9
Caelo	Polysorbate 80	12116014	1
Caelo	Polysorbate 80	123125308	1
Caelo	Polysorbate 80	12315305	1
Alliance Healthcare	Polysorbate 80	12315308	1
phönix	Polysorbate 80	12315328	1
Fagron	Polysorbate 80	12K05-N04	4
gehe 28.12.2013	Polysorbate 80	13152216	3
Caelo	Polysorbate 80	13152219	1
Fagron	Polysorbate 80	13A10-N03	2
Krieger	Polysorbate 80	131522232x	1
Fagron	Polysorbate 80	13C19-N01	1
Fagron	Polysorbate 80	13C19N01	1
Noweda	Polysorbate 80	13A10-N03	1
Caelo	Polysorbate 80	20210312-2	1
Caelo	Polysorbate 80	27111308	1
Caelo	Polysorbate 80	2772013	1
Caelo	Polysorbate 80	21061301	1
Sanacorp	Polysorbate 80	7/AKD20	1
Caelo	Polysorbate 80	Ch12116005	1
Fagron	Polysorbate 80	12D02-N02	1
Gehe	Polysorbate 80	12K05-N04	1
Caelo	Polysorbate 80	2915A-02527	1
Caelo	Polysorbate 80	4512A-02527	1
Caelo	Polysorbate 80	3212I-02527	1
Caelo	Polysorbate 80		1
Klenk	Polysorbate 80	12315328	1
Caelo	Polysorbate 80	3213E2527	1

- 58 233 spectra from 332 *Apo-Ident* customers from a total of 20 020 batches from a further 327 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 *Polysorbate 80 / Macrogolglycerolricinoleat* 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 *Polysorbate 80 / Macrogolglycerolricinoleat* 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	34 084
Type B	0	130	0	63 464
Type C	0	206	2	58 233

The substance/substance group *Polysorbate 80 / Macrogolglycerolricinoleat* 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 % (> 99.9689 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.5963 %)	99.0385 % (> 97.5962 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30766	31368	3.46	36.38
30893	31325	5.01	23.43
31015	31368	5.71	37.23
31325	31325	0.00	24.61
31368	31368	0.00	37.13

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Potash soap**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30987-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Potash soap; Sapo kalinus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Potash soap*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potash soap	13008101	30987	40	1402565
Caelo	Potash soap	13322201	31125	40	20131018
Caelo	Potash soap	14143401	31480	40	20140520
Caelo	Potash soap	14240801	31561	40	20140815
Caelo	Potash soap	14289101	31650	40	20141017

Validation samples

A total of 156 379 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 *Potash soap*. These samples are listed above in the [calibration samples](#) section.
- 34 144 spectra from a total of 793 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 200 spectra of 6 reference samples from the substance/substance group *Potash soap*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Potash soap	11136402	30336	40
Caelo	Potash soap	14240801	31561 [†]	20
Caelo	Potash soap	14289101	31650 [†]	20
Caelo	Potash soap	160908	32392	40
Caelo	Potash soap	160909	32393	40
Caelo	Potash soap	160910	32394	40

- 63 394 spectra from a total of 1471 batches from further 439 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.

- 28 spectra from 14 *Apo-Ident* customers from 23 batches from the substance/substance group *Potash soap*.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Potash soap	12060701	1
Caelo	Potash soap	11198901	1
Caelo	Potash soap	12060401	1
Caelo	Potash soap	11276401	1
Caelo	Potash soap	13161401	2
Caelo	Potash soap	13161901	2
Caelo	Potash soap	14033001	1
Caelo	Potash soap	13322601	1
Caelo	Potash soap	13322201	1
Caelo	Potash soap	14032901	1
Caelo	Potash soap	14240901	1
Caelo	Potash soap	14032801	1
Caelo	Potash soap	14241001	2
Caelo	Potash soap	14241101	2
Caelo	Potash soap	14289101	1
Caelo	Potash soap	14289201	1
Caelo	Potash soap	15/134/KS	1
Caelo	Potash soap	15182001	1
Caelo	Potash soap	15240401	1
Caelo	Potash soap	16091201	1
Caelo	Potash soap	15435201	1
Caelo	Potash soap	15240501	2
Caelo	Potash soap	16091101	1

- 58 413 spectra from 332 *Apo-Ident* customers from a total of 20 069 batches from a further 328 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 *Potash soap* 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 *Potash soap* 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	34 144
Type B	0	158	42	63 394
Type C	0	24	4	58 413

The substance/substance group *Potash soap* 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 % (> 99.9690 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9710 %)	79.0000 % (> 77.5000 %)
Type C	100.0000 % (> 99.5966 %)	85.7143 % (> 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.

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
30987	30987	0.00	59.06
31125	30987	28.56	53.32
31480	30987	11.97	56.64
31561	30987	12.48	58.13
31650	30987	15.50	60.00

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Propolis liquid extract 10% (in propylene glycol)
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30620-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Propolis liquid extract 10% (in propylene glycol)

Special notes

When selecting the *Propolis liquid extract 10% (in propylene glycol)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Propolis liquid extract 10% (in propylene glycol)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Propolis liquid ...	11220406	30620	40	20110829
Caelo	Propolis liquid ...	13347602	31195	40	1404589
Caelo	Propolis liquid ...	13347606	31458	40	20131030

Validation samples

A total of 156 379 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 *Propolis liquid extract 10% (in propylene glycol)*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Propolis liquid extract 10% (in propylene glycol)*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propolis liquid extract 10% ...	11220411	30612	40
Caelo	Propolis liquid extract 10% ...	13347606	31458 [†]	20

- 63 534 spectra from a total of 1475 batches from further 439 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 *Propolis liquid extract 10% (in propylene glycol)*.

Supplier	Substance	Batch	Spectra
Caelo	Propolis liquid extract 10% ...	14377411	1
Caelo	Propolis liquid extract 10% ...	12086105	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
Caelo	Propolis liquid extract 10% ...	12086102	1
Caelo	Propolis liquid extract 10% ...	13347601	1

- 58 437 spectra from 332 *Apo-Ident* customers from a total of 20 088 batches from a further 328 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 *Propolis liquid extract 10% (in propylene glycol)* 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 *Propolis liquid extract 10% (in propylene glycol)* 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	34 224
Type B	0	60	0	63 534
Type C	0	4	0	58 437

The substance/substance group *Propolis liquid extract 10% (in propylene glycol)* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.5985 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30620	31195	4.70	20.70
31195	31195	0.00	22.87
31458	31195	5.35	19.81

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Propylene glycol
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30872-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Propylene glycol; Propylenglycolum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Propylene glycol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Propylene glycol	12372405	30872	40	20130107
Henry Lamotte	Propylene glycol	0123095	30920	40	1502554
Caelo	Propylene glycol	14346604	31663	40	1508143
Euro OTC	Propylene glycol	1509031	31738	45	20151005*
Caelo	Propylene glycol	15335403	32074	40	20150930
Caelo	Propylene glycol	15355108	32486	40	20151021
Bombastus	Propylene glycol	301162	32728	40	20160323

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 285 spectra of 7 reference samples from the substance/substance group *Propylene glycol*. These samples are listed above in the [calibration samples](#) section.
- 34 059 spectra from a total of 791 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 155 spectra of 5 reference samples from the substance/substance group *Propylene glycol*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propylene glycol	14346604	31663 [†]	20
Euro OTC	Propylene glycol	1509031	31738 [†]	15
Euro OTC	Propylene glycol	1603034	32190	40
Euro OTC	Propylene glycol	1606014	32466	40
Euro OTC	Propylene glycol	1610031	32836	40

- 63 439 spectra from a total of 1472 batches from further 439 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.

*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.

[†]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*.

- 1719 spectra from 274 *Apo-Ident* customers from 330 batches from the substance/substance group *Propylene glycol*.

Supplier	Substance	Batch	Spectra
Fagron	Propylene glycol	16C10-B04-319299	1
Fagron	Propylene glycol	12J04-N06	11
Caelo	Propylene glycol	12169803	11
Sanacorp	Propylene glycol	123095	3
Caelo	Propylene glycol	1071502	1
Henry Lamotte/Phoenix	Propylene glycol	123095	11
HenryLamotteOilsGmbH	Propylene glycol	123095	1
Großhandel	Propylene glycol	123095	23
Lamotte Oils GmbH	Propylene glycol	123095	1
Lamotte/ Finze	Propylene glycol	123095	8
Henry Lamotte Oils GmbH...	Propylene glycol	123095	1
Caelo	Propylene glycol	125099	6
Henry Lamotte	Propylene glycol	125099	12
Euro OTC	Propylene glycol	125099	9
Sanacorp	Propylene glycol	125099	5
Henry/Geibo	Propylene glycol	125099	1
Henry Lamotte Oils / No...	Propylene glycol	125099	2
Henry Lamotte Oils GmbH...	Propylene glycol	125099	1
Henry Lamotte Oils GmbH	Propylene glycol	125099	1
Phoenix	Propylene glycol	125099	1
Caelo	Propylene glycol	2310070	1
Phoenix	Propylene glycol	29722B	1
Hedinger	Propylene glycol	29702B	1
Hedinger/ Sanacorp	Propylene glycol	29743B	1
Hedinger/Alliance Heath...	Propylene glycol	29775B	1
Hedinger/Sanacorp	Propylene glycol	29762B	2
Caelo	Propylene glycol	29814B	1
Caelo	Propylene glycol	3071402	1
Hedinger/Sanacorp	Propylene glycol	29823B	1
Hedinger	Propylene glycol	29797B	2
Fagron	Propylene glycol	50515PJK01	1
Hedinger	Propylene glycol	29775B	1
Fagron	Propylene glycol	8021621	1
Caelo	Propylene glycol	514E-02110	1
Henry Lamotte	Propylene glycol	1000001132	8
Lamotte/Anzag11	Propylene glycol	1000001132	3
Henry Lamotte Oils GmbH...	Propylene glycol	10000001132	1
Caelo	Propylene glycol	8051503	1
Caelo	Propylene glycol	1000001132	5
Henry Lamotte Oils GmbH	Propylene glycol	1000001132	4
Henry Lamotte Oils / No...	Propylene glycol	1000001132	1
Phoenix	Propylene glycol	1000001132	1
Lamotte	Propylene glycol	1000001132	1
Caelo	Propylene glycol	1113102	1
Phönix	Propylene glycol	114113102	1
Caelo	Propylene glycol	12071403	1
Fagron	Propylene glycol	1304C009	3
Caelo	Propylene glycol	1000002768	1
Fagron	Propylene glycol	1304C009-281100	3
Fagron	Propylene glycol	1307021-01	1
Euro OTC	Propylene glycol	1307021-01	9
Noweda 29.09.2014	Propylene glycol	1304C010-281099	1
Caelo	Propylene glycol	13111405	1
Caelo	Propylene glycol	13256704	22
Fagron	Propylene glycol	1314Q2110	1
Caelo	Propylene glycol	13256705	17
Noweda	Propylene glycol	13256705	3

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Supplier	Substance	Batch	Spectra
GEHE 06.05.2014	Propylene glycol	13256705	2
Caesar & Loretz GmbH Hi...	Propylene glycol	13256705	1
Caelo	Propylene glycol	13256706	20
Sanacorp	Propylene glycol	13256706	1
Caelo	Propylene glycol	13256707	27
Caelo	Propylene glycol	13256708	11
Caelo	Propylene glycol	13256709	14
Fagron	Propylene glycol	13E22-B03	9
Phoenix am 10.03.2014	Propylene glycol	13256709	1
Caelo	Propylene glycol	13E22-B03	1
Fagron	Propylene glycol	13E22-B03-283450	19
Phoenix	Propylene glycol	13E22B03283450	1
Fagron	Propylene glycol	13G09-B01-283456	17
Fagron	Propylene glycol	13E22-B03-28350	1
Fagron	Propylene glycol	13G09-B01	3
Fagron	Propylene glycol	13G09B01	2
Caelo	Propylene glycol	13G09-B01283456	1
Fagron	Propylene glycol	13G09B01283456	1
gehe	Propylene glycol	1401010-01	2
Euro OTC	Propylene glycol	1401010-01	7
Caelo	Propylene glycol	140101001	2
EuRho/Noweda	Propylene glycol	140020-01	1
Euro OTC	Propylene glycol	140500301	3
Fagron	Propylene glycol	1405003-01	1
Caelo	Propylene glycol	1405003-01	1
Euro OTC	Propylene glycol	1405003-01	2
Phönix 4.3.15	Propylene glycol	1405003-01	1
Caelo	Propylene glycol	14051802	15
Caelo	Propylene glycol	140510804	1
Gehe	Propylene glycol	14051802	1
Caelo	Propylene glycol	14051803	7
Caelo	Propylene glycol	14051804	10
Caesar & Loretz GmbH	Propylene glycol	14051804	2
Caelo	Propylene glycol	14051805	15
Euro OTC	Propylene glycol	1408020-01	9
Phoenix	Propylene glycol	14051805	1
Euro OTC	Propylene glycol	140802001	1
Caelo	Propylene glycol	14113102	16
Phönix	Propylene glycol	141113102	1
Phönix	Propylene glycol	14113102	1
Caelo	Propylene glycol	14113103	5
Sanacorp	Propylene glycol	14113103	1
Caelo	Propylene glycol	14113105	10
Alliance 05.2.15	Propylene glycol	14113105	1
Caelo	Propylene glycol	14248702	9
Caelo	Propylene glycol	1424870	1
Caelo	Propylene glycol	14248703	16
Sanacorp	Propylene glycol	14248703	1
Euro/ Sanacorp	Propylene glycol	14248704	1
Caelo	Propylene glycol	14248704	6
Caesar & Loretz GmbH Hi...	Propylene glycol	14248706	1
Caelo	Propylene glycol	14248706	5
Sanacorp	Propylene glycol	14248706	1
Caelo	Propylene glycol	14248707	12
Caesar & Loretz GmbH Hi...	Propylene glycol	14248707	1
Caelo	Propylene glycol	1428704	2
Caelo	Propylene glycol	14346603	8
Euro OTC	Propylene glycol	14346602	2
Caelo	Propylene glycol	1428706	1
Caelo	Propylene glycol	14346602	3

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Supplier	Substance	Batch	Spectra
Gehe	Propylene glycol	14346602	1
Caelo	Propylene glycol	14346604	5
Caelo	Propylene glycol	14346606	9
Caelo	Propylene glycol	14346605	2
Caelo	Propylene glycol	14346607	14
Caelo	Propylene glycol	14346608	6
Caelo	Propylene glycol	14346609	11
Caelo	Propylene glycol	1436604	1
Fagron	Propylene glycol	14A09-B04	13
Fagron	Propylene glycol	14A09B04	4
Fagron	Propylene glycol	14A09-B04-289597	11
Gehe	Propylene glycol	14A09-B04-289597	2
Phoenix	Propylene glycol	14a09-b04-289597	1
Phoenix	Propylene glycol	14A09-B04-289597	1
Fagron	Propylene glycol	14A09-B04-289598	2
Fagron	Propylene glycol	14A09-B04-289599	4
Fagron	Propylene glycol	14C05-B02	3
Fagron	Propylene glycol	14C05-B02-295787	4
Fagron	Propylene glycol	14A09-B04-289600	1
Phönix Gotha	Propylene glycol	14C05-B02-295787	1
Gehe 3.3.15	Propylene glycol	14C05-B02-295787	1
Fagron	Propylene glycol	14C05B02295787	2
Fagron	Propylene glycol	14C05-B02-295788	3
Fagron	Propylene glycol	14H22-B02-302506	5
BASF AG.	Propylene glycol	1501013-01	1
Euro OTC	Propylene glycol	1501013-01	9
Euro OTC	Propylene glycol	150101301	2
Euro OTC	Propylene glycol	1504031-01	13
Euro OTC	Propylene glycol	150403101	3
Euro OTC	Propylene glycol	15040301-01	1
EuRho/Noweda	Propylene glycol	1504031-01	1
Caelo	Propylene glycol	15069201	4
Caelo	Propylene glycol	15069202	12
Caelo	Propylene glycol	15081501	1
Euro OTC	Propylene glycol	1509031-01	10
EuRho	Propylene glycol	1509031-01	2
Caelo	Propylene glycol	150903101	1
Caelo	Propylene glycol	15181601	9
Euro OTC	Propylene glycol	150903101	1
Caelo	Propylene glycol	15181602	8
Caelo	Propylene glycol	15181603	12
Caelo	Propylene glycol	15181604	7
Caelo	Propylene glycol	15181605	6
Caesar&Loretz GmbH/Anzag	Propylene glycol	15181605	2
Caelo	Propylene glycol	151816055	1
Caelo	Propylene glycol	15262401	8
Caelo	Propylene glycol	15262402	4
Caelo	Propylene glycol	15262403	7
Noweda	Propylene glycol	15262402	1
Euro OTC	Propylene glycol	15262403	1
Caesar & Loretz GmbH	Propylene glycol	15262403	1
Caelo	Propylene glycol	15262404	8
Caelo	Propylene glycol	15262406	4
Caelo	Propylene glycol	15262407	5
Fagron	Propylene glycol	15262407	1
Caelo	Propylene glycol	15262408	7
Caelo	Propylene glycol	15262409	6
Caelo	Propylene glycol	1526407	1
Caelo	Propylene glycol	1533405	1
Caelo	Propylene glycol	15335403	6

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH Hi...	Propylene glycol	15335403	1
Caesar & Loretz GmbH Hi...	Propylene glycol	15335404	1
Beiersdorf AG	Propylene glycol	15335404	1
Sanacorp	Propylene glycol	15335404	1
Caelo	Propylene glycol	15335404	10
Caelo	Propylene glycol	15335405	10
Noweda	Propylene glycol	15335405	1
Caesar&Loretz GmbH	Propylene glycol	15335405	1
Caelo	Propylene glycol	15335406	13
Caelo	Propylene glycol	15335407	10
Fagron	Propylene glycol	15335407	1
Caelo	Propylene glycol	15335408	7
Caelo	Propylene glycol	15355108	5
Caelo	Propylene glycol	15430502	4
Caelo	Propylene glycol	15430503	8
Caelo	Propylene glycol	15430504	5
Bombastus	Propylene glycol	15430504	2
Caelo	Propylene glycol	15430505	1
Caelo	Propylene glycol	15430506	6
Wolf-Apotheke	Propylene glycol	15430506	1
Caesar & Loretz GmbH Hi...	Propylene glycol	15430508	1
Caelo	Propylene glycol	15430513	3
Caelo	Propylene glycol	15430508	2
EuroPTC/Phönix	Propylene glycol	15901013-01	1
Alliance H.	Propylene glycol	15430513	1
Caelo	Propylene glycol	1562408	1
Caelo	Propylene glycol	15430514	2
Fagron	Propylene glycol	15A07B04	3
Fagron	Propylene glycol	15A07-B04	3
Fagron	Propylene glycol	15A07-B04-302969	4
Fagron	Propylene glycol	15A07-B04-302970	4
Phönix Gotha	Propylene glycol	15A07-B04-302970	2
Fagron	Propylene glycol	15B24-B40	1
Fagron	Propylene glycol	15B24-B40-307379	2
Caelo	Propylene glycol	15A07-B04-302970	1
Fagron	Propylene glycol	15F25-B02-311890	2
Fagron	Propylene glycol	15G28-B03	2
Fagron	Propylene glycol	15G28-B03-314768	2
Fagron	Propylene glycol	15L23-B01-318036	4
Caelo	Propylene glycol	16021506	1
Euro OTC	Propylene glycol	1603034	1
Euro OTC	Propylene glycol	1603034-01	9
Euro OTC	Propylene glycol	160303401	1
Euro OTC	Propylene glycol	1606014-01	2
Caelo	Propylene glycol	16105403	9
Calo/Sanacorp	Propylene glycol	16105403	1
Caelo	Propylene glycol	16251201	2
Caelo	Propylene glycol	16105404	1
Caelo	Propylene glycol	16251202	2
Fagron	Propylene glycol	16C10-B04	1
Fagron	Propylene glycol	16E09-B02-324843	2
Fagron	Propylene glycol	16C10-B04-323302	1
Caelo	Propylene glycol	1793451	3
Fagron	Propylene glycol	17082015A	1
Caelo	Propylene glycol	17041501	1
Apotheke-Ansatz	Propylene glycol	19/15	1
Caelo	Propylene glycol	26021320	2
Fagron	Propylene glycol	18061321	2
Fagron	Propylene glycol	18061311	1
Caelo	Propylene glycol	26041402	1

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Supplier	Substance	Batch	Spectra
Caelo	Propylene glycol	27091402	2
Caelo	Propylene glycol	28071503	1
Bombastus	Propylene glycol	289078	5
Bombastus	Propylene glycol	286382	4
Bombastus	Propylene glycol	291103	1
Caelo	Propylene glycol	29091403	1
Bombastus	Propylene glycol	293947	7
Bombastus	Propylene glycol	295111	3
Bombastus	Propylene glycol	296424	1
Bombastus	Propylene glycol	297626	2
Bombastus	Propylene glycol	299106	4
Bombastus	Propylene glycol	301162	4
Bombastus	Propylene glycol	303788	2
Caelo	Propylene glycol	31256708	1
Sanacorp	Propylene glycol	49/AKD1	1
Caelo	Propylene glycol	4248702	1
Henry Lamotte Oils GmbH	Propylene glycol	5471401	1
Fagron	Propylene glycol	5115Q-02110	1
Sanacorp	Propylene glycol	50/AKD3	1
Caelo	Propylene glycol	5262402	1
Lamotte	Propylene glycol	5671401	8
Henry Lamotte Oils GmbH	Propylene glycol	5671401	8
Henry Lamotte Oils GmbH...	Propylene glycol	5671401	1
lamotte	Propylene glycol	5671401	2
Henry Lamotte/Anzag	Propylene glycol	5671401	2
Caelo	Propylene glycol	5671401	7
Lamotte / Alliance Heal...	Propylene glycol	5671401	1
Sanacorp	Propylene glycol	5671401	1
Sanacorp	Propylene glycol	AKD70	1
Caelo	Propylene glycol	6509HH9041	1
Caelo	Propylene glycol	83/2014	1
Bombastus	Propylene glycol	265358	1
Bombastus	Propylene glycol	270359	1
Caelo	Propylene glycol		2
Bombastus	Propylene glycol	268295	1
Caelo	Propylene glycol	113Q-02110	1
Bombastus	Propylene glycol	7/14	1
Celo	Propylene glycol	11607-2	1
Lamotte 004	Propylene glycol	122882	1
Lamotte	Propylene glycol	122690	1
Großhandel	Propylene glycol	122882	1
Noweda / Henry Lamotte	Propylene glycol	122882	1
Henry Lamotte,Phönix	Propylene glycol	123095	2
Henry Lamotte	Propylene glycol	123095	4
Henry Lamotte Oils GmbH	Propylene glycol	123095	2
Bombastus	Propylene glycol	123095	1
Henry Lamotte oils GmbH	Propylene glycol	123095	1
Henry Lam./ Phönix	Propylene glycol	123095	1
henry lamotte	Propylene glycol	125099	1
Caelo	Propylene glycol	2101302	1
Hedinger	Propylene glycol	29625B	1
Hedinger	Propylene glycol	29595B	1
Fagron	Propylene glycol	9051220	7
Caelo	Propylene glycol	5061201	1
Caelo	Propylene glycol	6021301	1
Fagron	Propylene glycol	8121120	1
Caelo	Propylene glycol	611211	1
Fagron	Propylene glycol	9031321	1
Henry Lamotte Oils	Propylene glycol	7021401	1
Caelo	Propylene glycol	70214PJK02	1

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Supplier	Substance	Batch	Spectra
henry lamotte	Propylene glycol	1000001132	1
Euro OTC	Propylene glycol	1109015-01	1
Phönix Gotha	Propylene glycol	10210312	1
Alliance Healthcare	Propylene glycol	10274303	1
Caelo	Propylene glycol	11021404	1
Noweda	Propylene glycol	1112004-01	2
Caelo	Propylene glycol	10274305	2
Caelo	Propylene glycol	10210307	1
Caelo	Propylene glycol	10371307	1
Caelo	Propylene glycol	11125812	1
Caelo	Propylene glycol	11125811	1
Caelo	Propylene glycol	11300502	2
Caelo	Propylene glycol	11125804	1
Gehe	Propylene glycol	11300506	1
Caesar & Loretz GmbH, 4...	Propylene glycol	11300505	1
Caelo	Propylene glycol	11300506	5
Kehr	Propylene glycol	11300506	1
Caelo	Propylene glycol	11300505	1
Phönix	Propylene glycol	1130505	1
Noweda	Propylene glycol	11300506	1
Euro OTC	Propylene glycol	1136HH9041	1
Caelo	Propylene glycol	11372005	3
Noweda	Propylene glycol	11372005	2
Caelo	Propylene glycol	11372006	15
noweda	Propylene glycol	11372006	1
Erika apotheke	Propylene glycol	11372006	1
Caesar & Loretz GmbH	Propylene glycol	11372006	1
Caelo	Propylene glycol	11372007	7
Noweda	Propylene glycol	11372007	1
Fagron	Propylene glycol	11372007	2
Caesar & Loretz GmbH, 4...	Propylene glycol	11372007	1
Phönix 28.08.2012	Propylene glycol	11372007	1
Gehe	Propylene glycol	11372007	3
Caelo	Propylene glycol	11372009	5
Noweda	Propylene glycol	11372009	1
Gehe	Propylene glycol	11372009	1
Caelo	Propylene glycol	11372010	6
Caelo	Propylene glycol	11372011	4
Fagron	Propylene glycol	11H04-N01	3
Phönix Gotha	Propylene glycol	11372011	1
Euro OTC	Propylene glycol	11C07-N06	1
Fagron	Propylene glycol	11F10-N04	1
v.d.l	Propylene glycol	11h04-n01	1
Caelo	Propylene glycol	11H04-N01	1
Fagron	Propylene glycol	11K28-N01	9
Caelo	Propylene glycol	11K28-N01	1
Fagron	Propylene glycol	11L22-N14	7
Sanacorp	Propylene glycol	1206038-01	1
Euro OTC	Propylene glycol	1206038-01	3
Caelo	Propylene glycol	1206038-01	1
Euro OTC	Propylene glycol	120603801	1
Noweda	Propylene glycol	12088205	3
Caelo	Propylene glycol	12088205	3
Fagron	Propylene glycol	12088205	1
Herbasinica	Propylene glycol	12088206	2
Caelo	Propylene glycol	12088207	15
Caelo	Propylene glycol	12088206	4
Phytocomm	Propylene glycol	12088207	1
Noweda	Propylene glycol	12088207	2
Caelo	Propylene glycol	1208827	1

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Supplier	Substance	Batch	Spectra
Eigenherstellung	Propylene glycol	120912PML01	1
Fagron	Propylene glycol	120C004-277798	1
Caelo	Propylene glycol	12111304	1
Caesar & Loretz GmbH, 4...	Propylene glycol	12169802	5
Caelo	Propylene glycol	12100907	1
Caelo	Propylene glycol	12169802	15
Anzag 25.01.2013	Propylene glycol	12169802	2
Noweda	Propylene glycol	12169802	2
Gehe	Propylene glycol	12169802	1
Caelo	Propylene glycol	12169804	8
Caelo	Propylene glycol	12372402	2
Alliance Healthcare	Propylene glycol	12372403	1
Caelo	Propylene glycol	12372403	7
Fagron	Propylene glycol	12372403	1
Caelo	Propylene glycol	12372404	13
Anzag 19.03.13 ek: 3,03EUR	Propylene glycol	12372404	2
Caesar & Loretz GmbH	Propylene glycol	12372404	1
Caelo	Propylene glycol	12372405	15
Gehe	Propylene glycol	12372405	2
Gehe 00.07.2013	Propylene glycol	12372405	1
Phönix	Propylene glycol	12372405	1
Caelo	Propylene glycol	1288205	1
Fagron	Propylene glycol	12C06-N04	6
Caelo	Propylene glycol	12C06-N04	1
Fagron	Propylene glycol	12G13-N07	29
Fagron	Propylene glycol	12g13-n07	3
Caelo	Propylene glycol	12G13-N07	1
Fagron	Propylene glycol	12G13-N07	5
Gehe	Propylene glycol	12J04-N06	2
Fagron	Propylene glycol	12G13-No7	1
Gehe	Propylene glycol	12K13-N05	2
Fagron	Propylene glycol	12K13-N05	15
Fagron	Propylene glycol	12k13-n05	2
Caelo	Propylene glycol	12K13-N05	1
Fargon	Propylene glycol	12K13-N05	2
Fagron	Propylene glycol	1301C003	2
Fagron	Propylene glycol	1301C003-277799	1
Fagron	Propylene glycol	1301C004	5
Fagron	Propylene glycol	1301C004-277798	18
Phönix Gotha	Propylene glycol	1301C004-277798	1
Phoenix	Propylene glycol	1301C004-277798	1
EuRho	Propylene glycol	1302002-01	1
Euro OTC	Propylene glycol	1302002-01	11
Noweda	Propylene glycol	1302002-01	1
Fagron	Propylene glycol	13040010-281099	1
Euro OTC	Propylene glycol	130200201	2
Caelo	Propylene glycol	1304C009-281100	2
Fagron	Propylene glycol	1304C009-28	1
Fagron	Propylene glycol	1304C010	9
Fagron	Propylene glycol	1304C-010	1
Fagron	Propylene glycol	1304C010-281099	14
Gehe	Propylene glycol	1304C010-281099	2
Fagron	Propylene glycol	1304C010281099	1
Phoenix	Propylene glycol	1304C010-281099	1
Fagron	Propylene glycol	1304C010	1
Euro OTC	Propylene glycol	130702101	1
Caelo	Propylene glycol	13071303	1
Caelo	Propylene glycol	13100906	11
Caesar/Noweda	Propylene glycol	13100906	1
Caelo	Propylene glycol	13100907	19

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Supplier	Substance	Batch	Spectra
AHD	Propylene glycol	13100907	1
Phoenix	Propylene glycol	13100907	1
Cealo	Propylene glycol	13100907	2
Caelo	Propylene glycol	13100908	33
Gehe	Propylene glycol	13100908	3
Caelo	Propylene glycol	1316003	1
Caesar /phönix	Propylene glycol	13167003	1
Noweda	Propylene glycol	1313HH9041	1
Caelo	Propylene glycol	13167003	23
Caelo	Propylene glycol	1310098	1
Noweda	Propylene glycol	13167003	1
canea, anzag	Propylene glycol	13167003	3
Phönix	Propylene glycol	13167003	2
Gehe	Propylene glycol	13167003	2
Caelo	Propylene glycol	13167004	25
Phönix	Propylene glycol	13167004	1
Caelo	Propylene glycol	13167006	7
Caelo	Propylene glycol	13167005	1
Phönix	Propylene glycol	13167006	1
Caesar/Noweda	Propylene glycol	13167006	2
Sanacorp	Propylene glycol	13167006	1
Noweda	Propylene glycol	13256704	1
Gehe	Propylene glycol	13256704	2
ANZAG 20.01.2014	Propylene glycol	13256704	1
Phoenix	Propylene glycol	13256705	1
Fagron	Propylene glycol	13E22B03	1
Fagron	Propylene glycol	13E22B0328345	1
gehe	Propylene glycol	13E22-B03-283450	1
Fagron	Propylene glycol	13E22-B03-283451	2
Euro OTC	Propylene glycol	140101001	1
Fagron	Propylene glycol	14051802	2
Caesar/Noweda	Propylene glycol	14051803	1
Phönix	Propylene glycol	14248706	1
Caelo	Propylene glycol	150771	1
Caesar&lloretz,Phoenix	Propylene glycol	15069202	1
Phoenix	Propylene glycol	18061321	1
Caelo	Propylene glycol	1804212110	1
Caelo	Propylene glycol	18041302	1
Fagron	Propylene glycol	18081121	2
Fischbar	Propylene glycol	18091201	1
Gehe	Propylene glycol	18081121	1
Fagron	Propylene glycol	181013prop	1
Caelo	Propylene glycol	20140612-6	1
Caelo	Propylene glycol	19041307	1
Caelo	Propylene glycol	24041221	2
Caelo	Propylene glycol	20071201	1
Fagron	Propylene glycol	2112212110	1
Caelo	Propylene glycol	20111203	1
Fagron	Propylene glycol	24041221	9
Gehe	Propylene glycol	24041221	1
Caelo	Propylene glycol	25011302	1
Caelo	Propylene glycol	24121301	1
Caelo	Propylene glycol	25031301	1
Fagron	Propylene glycol	26021320	3
Alliance Healthcare	Propylene glycol	272684	1
Caelo	Propylene glycol	26061302	1
Bombastus	Propylene glycol	277548	4
Bombastus	Propylene glycol	281569	3
Caelo	Propylene glycol	28021301	1
Bombastus	Propylene glycol	283937	1

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Supplier	Substance	Batch	Spectra
Fagron	Propylene glycol		2
Caelo	Propylene glycol	2913M-02110	1
Caelo	Propylene glycol	3512M-02110	1
Caelo	Propylene glycol	42488055	1
Caelo	Propylene glycol	31051317	1
Henry Lamotte	Propylene glycol	5671401	1
Phagron	Propylene glycol		1
Gehe	Propylene glycol	Test2	1
Phönix	Propylene glycol	Retest03083	1
Caelo	Propylene glycol	Ch13100908	1
Fagron	Propylene glycol	Ch12J04-N06	1
phönix	Propylene glycol	AKD30	1
Henry Lamotte Oils	Propylene glycol	123095	3
Henry Lamotte Oils	Propylene glycol	122880	1
Caelo	Propylene glycol	122882	1
Phönix	Propylene glycol	29595B	1
A.H.D.	Propylene glycol	1112004-01	1
Caelo	Propylene glycol	11300504	1
GEHE	Propylene glycol	11372007	1
Fagron	Propylene glycol	11h04-n01	1
Gehe	Propylene glycol	12088207	1
Anzag	Propylene glycol	12G13N07	1
Caelo	Propylene glycol	1301C003-277799	1
Caelo	Propylene glycol	1301c004	2
Fagron	Propylene glycol	1301C004-0005	1
Sanacorp	Propylene glycol	1302002-01	1
Fagron	Propylene glycol	1304c009-281100	1
Fagron	Propylene glycol	1304c010-281099	1
Caelo	Propylene glycol	13100905	2
Fagron	Propylene glycol	13G09-B01-283452	1
Fagron	Propylene glycol	o903132121	1

- 56 722 spectra from 332 *Apo-Ident* customers from a total of 19 766 batches from a further 328 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 *Propylene glycol* 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 *Propylene glycol* 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	285	0	34 059
Type B	0	155	0	63 439
Type C	0	1695	24	56 722

The substance/substance group *Propylene glycol* 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 % (> 99.9689 %)	100.0000 % (> 97.8947 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 96.1290 %)
Type C	100.0000 % (> 99.5963 %)	98.6038 % (> 98.4293 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30872	31663	3.43	24.18
30920	30920	0.00	22.73
31663	31663	0.00	26.25
31738	31738	0.00	22.11
32074	31663	5.51	28.57
32486	31663	6.76	32.61
32728	31663	5.57	21.99

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Psorisol base cream Audor®
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31109-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Psorisol base cream Audor®

Special notes

When selecting the *Psorisol base cream Audor®* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Psorisol base cream Audor®*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor	Psorisol base cr...	AP101943PB	31109	40	1404015
Audor	Psorisol base cr...	AP101943PB	31233	40	20130522
Audor	Psorisol base cr...	AP45001.2PB	31674	40	20141230
Audor	Psorisol base cr...	AP55201PB	32275	40	20160204

Validation samples

A total of 156 379 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 *Psorisol base cream Audor®*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 100 spectra of 3 reference samples from the substance/substance group *Psorisol base cream Audor®*.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Psorisol base cream Audor®	AP102640PB	30281	40
Audor Pharma	Psorisol base cream Audor®	AP45001.2PB	31674 [†]	20
Audor Pharma	Psorisol base cream Audor®	AP45001.2PB	32274	40

- 63 494 spectra from a total of 1475 batches from further 439 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 8 *Apo-Ident* customers from 12 batches from the substance/substance group *Psorisol base cream Audor®*.

Supplier	Substance	Batch	Spectra
Audor Pharma	Psorisol base cream Audor®	102844	2

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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
Audor Pharma	Psorisol base cream Audor [®]	101943	1
Audor Pharma	Psorisol base cream Audor [®]	AP55201PB	4
Caelo	Psorisol base cream Audor [®]	AP102844PB	2
Audor Pharma	Psorisol base cream Audor [®]	AP101943PB	3
Audor Pharma	Psorisol base cream Audor [®]		1
Audor Pharma	Psorisol base cream Audor [®]	102891	1
Audor Pharma	Psorisol base cream Audor [®]	AP102844PB	1
Audor Pharma	Psorisol base cream Audor [®]	102891PB	1
Audor Pharma	Psorisol base cream Audor [®]	AP11943PB	1
Audor Pharma	Psorisol base cream Audor [®]	AP100472PB	2
Audor Pharma	Psorisol base cream Audor [®]	AP102891PB	1
Anzag	Psorisol base cream Audor [®]	AP102891PB	2

- 58 419 spectra from 332 *Apo-Ident* customers from a total of 20 080 batches from a further 328 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 *Psorisol base cream Audor[®]* 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 *Psorisol base cream Audor[®]* 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	34 184
Type B	0	100	0	63 494
Type C	0	20	2	58 419

The substance/substance group *Psorisol base cream Audor[®]* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.5967 %)	90.9091 % (> 77.2727 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31109	31109	0.00	23.25
31233	31109	4.38	22.96
31674	31109	4.40	23.72
32275	31109	6.13	23.59

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Raspberry aroma**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30562-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Raspberry aroma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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	20140416
Caelo	Raspberry aroma	16126605	33222	40	20160421

Validation samples

A total of 156 379 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 *Raspberry aroma*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Raspberry aroma*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Raspberry aroma	11303813	30562	40
Caelo	Raspberry aroma	12054307	30611	40

- 63 514 spectra from a total of 1475 batches from further 439 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 23 *Apo-Ident* customers from 25 batches from the substance/substance group *Raspberry aroma*.

Supplier	Substance	Batch	Spectra
Caelo	Raspberry aroma	13255514	3
Caelo	Raspberry aroma	13255507	2
Caelo	Raspberry aroma	1355514	1
Caelo	Raspberry aroma	14115902	2
Caelo	Raspberry aroma	14115913	2
Caelo	Raspberry aroma	14376103	2

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Supplier	Substance	Batch	Spectra
Caelo	Raspberry aroma	14376115	1
Caelo	Raspberry aroma	14378103	1
Caelo	Raspberry aroma	15219102	2
Caelo	Raspberry aroma	15438503	1
Caelo	Raspberry aroma	15438501	2
Caelo	Raspberry aroma	11303813	1
Rondell Apotheke	Raspberry aroma	15438501	1
Caelo	Raspberry aroma	12054302	1
Caelo	Raspberry aroma	16126605	1
Gehe 16.04.2013	Raspberry aroma	12054307	1
Caelo	Raspberry aroma	12246608	1
Caelo	Raspberry aroma	12246604	1
Phönix Gotha	Raspberry aroma	12246612	1
Caelo	Raspberry aroma	12246612	2
Caelo	Raspberry aroma	12054310	2
Caelo	Raspberry aroma	12246616	2
Caelo	Raspberry aroma	12246617	1
Caelo	Raspberry aroma	1254307	1
Caelo	Raspberry aroma	13255502	2
Caelo	Raspberry aroma	12054311	1
Caelo	Raspberry aroma	14115909	1

- 58 402 spectra from 332 *Apo-Ident* customers from a total of 20 067 batches from a further 328 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	120	0	34 224
Type B	0	80	0	63 514
Type C	0	38	1	58 402

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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5965 %)	97.4359 % (> 89.7436 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31171	31171	0.00	66.69
31396	31171	4.54	67.33
33222	31171	5.67	73.49

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Rose oil (genuine / artificial)**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30111-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Rose oil (genuine / artificial); Oleum rosae (verum / artificiale)

Special notes

When selecting the *Rose oil (genuine / artificial)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 (genuine / artificial)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Rose oil (genuin...	12164308	31021	40	1502254
Caelo	Rose oil (genuin...	11287117	31022	40	20111011
Fagron	Rose oil (genuin...	13J17-B01	31290	40	1507614
Caelo	Rose oil (genuin...	13335012	31301	20	20131009
Caelo	Rose oil (genuin...	13252710	31412	40	1502252
Caelo	Rose oil (genuin...	13335012	31425	40	20131009
Fagron	Rose oil (genuin...	14I25-B01-302286	31752	40	20141006
Fagron	Rose oil (genuin...	14I25-B01-302286	31842	40	20141006

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 8 reference samples from the substance/substance group *Rose oil (genuine / artificial)*. These samples are listed above in the [calibration samples](#) section.
- 34 044 spectra from a total of 792 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 203 spectra of 6 reference samples from the substance/substance group *Rose oil (genuine / artificial)*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Rose oil (genuine / artifici...	9185909	30209	43
Caelo	Rose oil (genuine / artifici...	13335012	31425 [†]	20
Caelo	Rose oil (genuine / artifici...	13335012	31426	60
Fagron	Rose oil (genuine / artifici...	14I25-B01-302286	31752 [†]	20
Fagron	Rose oil (genuine / artifici...	14I25-B01-302286	31842 [†]	20
Caelo	Rose oil (genuine / artifici...	162311	32332	40

- 63 391 spectra from a total of 1473 batches from further 439 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.

- 85 spectra from 48 *Apo-Ident* customers from 43 batches from the substance/substance group *Rose oil (genuine / artificial)*.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Rose oil (genuine / artifici. ...)	11287114	1
Caelo	Rose oil (genuine / artifici. ...)	11287117	2
Fagron	Rose oil (genuine / artifici. ...)	7091301	1
Fargon	Rose oil (genuine / artifici. ...)	12H16-B01-286704	3
Fagron	Rose oil (genuine / artifici. ...)	12C19-N05	3
Fagron	Rose oil (genuine / artifici. ...)	12G25-N02	6
Phönix	Rose oil (genuine / artifici. ...)	13C21-N04	2
Fagron	Rose oil (genuine / artifici. ...)	13C21-N04	10
Fagron	Rose oil (genuine / artifici. ...)	12H16-B01-286704	3
Caelo	Rose oil (genuine / artifici. ...)	13252723	1
Caelo	Rose oil (genuine / artifici. ...)	13252710	2
Caelo	Rose oil (genuine / artifici. ...)	14300712	1
Fagron	Rose oil (genuine / artifici. ...)	14I25-B01	3
Fagron	Rose oil (genuine / artifici. ...)	12G25-N01	1
Caelo	Rose oil (genuine / artifici. ...)	15197202	5
Fagron	Rose oil (genuine / artifici. ...)	12H16-B01	2
Caelo	Rose oil (genuine / artifici. ...)	11287123	1
Caelo	Rose oil (genuine / artifici. ...)	13252722	2
Caelo	Rose oil (genuine / artifici. ...)	13252701	2
Caelo	Rose oil (genuine / artifici. ...)	1352710	1
Caelo	Rose oil (genuine / artifici. ...)	13335006	1
Fagron	Rose oil (genuine / artifici. ...)	13J17-801	1
Fagron	Rose oil (genuine / artifici. ...)	13C21-N074	1
Fagron	Rose oil (genuine / artifici. ...)	13J17-B01	2
Fagron	Rose oil (genuine / artifici. ...)	13J17-B01-293574	2
Fagron	Rose oil (genuine / artifici. ...)	14/25-B01-302286	1
Fagron	Rose oil (genuine / artifici. ...)	13J17-B01-296955	1
Fagron	Rose oil (genuine / artifici. ...)	1425-B01-302287	1
Caelo	Rose oil (genuine / artifici. ...)	14300703	1
Caelo	Rose oil (genuine / artifici. ...)	17101412	1
Caelo	Rose oil (genuine / artifici. ...)	19011502	1
Fagron	Rose oil (genuine / artifici. ...)	15/25-B01-302286	1
Fagron	Rose oil (genuine / artifici. ...)	1425-01-309676	1
Fagron	Rose oil (genuine / artifici. ...)	2188	1
Fagron	Rose oil (genuine / artifici. ...)	713371	1
Caelo	Rose oil (genuine / artifici. ...)	15G29-B12-314833	1
Caelo	Rose oil (genuine / artifici. ...)	11178601	1
Fagron	Rose oil (genuine / artifici. ...)	511I-02011	1
Fagron	Rose oil (genuine / artifici. ...)	11E04-N04	1
Caelo	Rose oil (genuine / artifici. ...)	13044608	2
Fagron	Rose oil (genuine / artifici. ...)	11H05-N02	1
Caelo	Rose oil (genuine / artifici. ...)	12164306	1
Phönix	Rose oil (genuine / artifici. ...)	12C19-N05	1
FARGON	Rose oil (genuine / artifici. ...)	12c19-n05	1
Phönix	Rose oil (genuine / artifici. ...)	12G25-N02	2
Gehe 29.06.2013	Rose oil (genuine / artifici. ...)	12G25-N02	1
Fagron	Rose oil (genuine / artifici. ...)	887963	1
Fagron	Rose oil (genuine / artifici. ...)	698884	2

- 58 356 spectra from 332 *Apo-Ident* customers from a total of 20 049 batches from a further 328 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 (genuine / artificial)* 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 (genuine / artificial)* 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	34 044
Type B	0	203	0	63 391
Type C	0	78	7	58 356

The substance/substance group *Rose oil (genuine / artificial)* 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 % (> 99.9689 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 97.0443 %)
Type C	100.0000 % (> 99.5964 %)	91.7647 % (> 88.2353 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31021	31021	0.00	86.25
31022	31412	9.79	64.39
31290	31290	0.00	266.02
31301	31021	9.73	79.62
31412	31412	0.00	60.16
31425	31021	5.66	81.51
31752	31290	3.40	275.66
31842	31290	3.70	276.93

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Sage oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30578-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sage oil; Oleum salviae; Salvia officinalis oleum

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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
Caelo	Sage oil	11287302	30578	40	1403165
Caelo	Sage oil	13146901	31597	40	20130522

Validation samples

A total of 156 379 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 *Sage oil*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 100 spectra of 3 reference samples from the substance/substance group *Sage oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sage oil	10248202	30170	40
Caelo	Sage oil	13146901	31597 [†]	20
Caelo	Sage oil	16051006	33265	40

- 63 494 spectra from a total of 1474 batches from further 439 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.

- 78 spectra from 48 *Apo-Ident* customers from 37 batches from the substance/substance group *Sage oil*.

Supplier	Substance	Batch	Spectra
Caelo	Sage oil	13146901	7
Caelo	Sage oil	13146914	4

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sage oil	13146907	1
Caelo	Sage oil	13146903	2
Caelo	Sage oil	13146908	2
Caelo	Sage oil	14345512	1
Caelo	Sage oil	10248206	2
Anzag, 11.09.2012	Sage oil	11287305	1
Caelo	Sage oil	11287306	1
Caelo	Sage oil	11287311	2
Caelo	Sage oil	10248215	1
Anzag 10.8.12 ek:4,42	Sage oil	11287305	1
Caelo	Sage oil	11287307	1
Caelo	Sage oil	11287312	1
Caelo	Sage oil	11287314	2
Caelo	Sage oil	11287315	1
Caelo	Sage oil	11287317	8
Caesar & Loretz GmbH, 4...	Sage oil	11287317	1
Caelo	Sage oil	11287318	1
Caelo	Sage oil	11287320	3
Gehe	Sage oil	11287318	1
Caelo	Sage oil	11287323	7
gehe	Sage oil	13146901	2
Caelo	Sage oil	13146904	1
Caelo	Sage oil	21111301	1
Caelo	Sage oil	14345517	2
Caelo	Sage oil	28051312	1
Sanacorp	Sage oil	282545	1
Caelo	Sage oil	31011401	1
Taoasis	Sage oil	498780-106211	1
Toasis	Sage oil	526975-110409	1
Taoasis	Sage oil	526975-111295	1
Taoasis GmbH	Sage oil	526975-110409	1
Taoasis	Sage oil	530771-108279	1
Caelo	Sage oil	5x11287317	1
Bombastus	Sage oil	298189	1
Bombastus	Sage oil	274447	1
Caelo	Sage oil	13146918	1
Caelo	Sage oil	1024214	1
Caelo	Sage oil	14345505	5
Caelo	Sage oil	14345511	2
Caelo	Sage oil	1435517	1

- 58 363 spectra from 332 *Apo-Ident* customers from a total of 20 055 batches from a further 328 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	80	0	34 264
Type B	0	50	50	63 494
Type C	0	61	17	58 363

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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9710 %)	50.0000 % (> 47.0000 %)
Type C	100.0000 % (> 99.5964 %)	78.2051 % (> 74.3590 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30578	30578	0.00	29.79
31597	30578	10.63	22.15

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Salicylic acid 50 % (paraffin)
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30496-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Salicylic acid 50 % (paraffin); Acidum salicylicum cum vaselino alba 50 %

Special notes

When selecting the *Salicylic acid 50 % (paraffin)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 acid 50 % (paraffin)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Salicylic acid 5...	12305902	30883	40	20121107
Henry Lamotte	Salicylic acid 5...	5375300	30927	40	20121003
Caelo	Salicylic acid 5...	15231801	31727	40	AR-15-FG-015411-01
Caelo	Salicylic acid 5...	153729	31901	40	20151029*
Caelo	Salicylic acid 5...	153730	31902	40	20151029*
Caelo	Salicylic acid 5...	153731	31903	40	20151103*
Henry Lamotte	Salicylic acid 5...	6001023001	32176	40	20150630
Caelo	Salicylic acid 5...	162761	32520	40	20160923*

Validation samples

A total of 156 379 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 *Salicylic acid 50 % (paraffin)*. These samples are listed above in the [calibration samples](#) section.
- 34 024 spectra from a total of 790 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 320 spectra of 9 reference samples from the substance/substance group *Salicylic acid 50 % (paraffin)*.

Supplier	Substance	Batch	Sample ID	Spectra
apomix	Salicylic acid 50 % (paraffin)	4B270911	30363	20
apomix	Salicylic acid 50 % (paraffin)	1A130212	30496	40
Caelo	Salicylic acid 50 % (paraffin)	14107901	31357	60
Caelo	Salicylic acid 50 % (paraffin)	15231801	31727 [†]	20
Caelo	Salicylic acid 50 % (paraffin)	153729	31901 [†]	20
Caelo	Salicylic acid 50 % (paraffin)	153730	31902 [†]	20
Caelo	Salicylic acid 50 % (paraffin)	153731	31903 [†]	20
Caelo	Salicylic acid 50 % (paraffin)	153732	31904	60
Caelo	Salicylic acid 50 % (paraffin)	153733	31905	60

- 63 274 spectra from a total of 1468 batches from further 439 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](#).

*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.

[†]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*.

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.

- 387 spectra from 131 *Apo-Ident* customers from 98 batches from the substance/substance group *Salicylic acid 50 % (paraffin)*.

Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid 50 % (paraffin)	15247101	12
Caelo	Salicylic acid 50 % (paraffin)	15231801	9
Caelo	Salicylic acid 50 % (paraffin)	15305901	10
Caelo	Salicylic acid 50 % (paraffin)	15305801	6
A.H.D.	Salicylic acid 50 % (paraffin)	1228301	1
HENRY LAMOTTE OILS GmbH	Salicylic acid 50 % (paraffin)	5375300	2
Phönix	Salicylic acid 50 % (paraffin)	12201801	1
Apomix / 11	Salicylic acid 50 % (paraffin)	1A180214	2
Apomix / 11	Salicylic acid 50 % (paraffin)	4A080515	1
Caelo	Salicylic acid 50 % (paraffin)		1
Noweda/apomix	Salicylic acid 50 % (paraffin)	5A020615	1
Apomix / Phönix	Salicylic acid 50 % (paraffin)	6B110714	1
Caelo	Salicylic acid 50 % (paraffin)	13278701	10
apomix	Salicylic acid 50 % (paraffin)	5A070416	1
Apomix / 11	Salicylic acid 50 % (paraffin)	10A181114	1
apomix	Salicylic acid 50 % (paraffin)	12A050916	1
Cealo	Salicylic acid 50 % (paraffin)	14017501	3
Caelo	Salicylic acid 50 % (paraffin)	14017501	13
Caelo	Salicylic acid 50 % (paraffin)	14107901	15
Apomix/Gehe	Salicylic acid 50 % (paraffin)	11A290716	1
Caelo	Salicylic acid 50 % (paraffin)	14108001	18
Caelo	Salicylic acid 50 % (paraffin)	14108301	3
Caelo	Salicylic acid 50 % (paraffin)	14204302	1
Raben-Apotheke Mildenau	Salicylic acid 50 % (paraffin)	14108201	1
Caelo	Salicylic acid 50 % (paraffin)	14108201	3
Caelo	Salicylic acid 50 % (paraffin)	14205101	5
Caelo	Salicylic acid 50 % (paraffin)	14337301	11
Caelo	Salicylic acid 50 % (paraffin)	14337201	8
Caelo	Salicylic acid 50 % (paraffin)	14354101	2
Caelo	Salicylic acid 50 % (paraffin)	15231601	5
Caelo	Salicylic acid 50 % (paraffin)	15373301	5
Lamotte/Gehe	Salicylic acid 50 % (paraffin)	5763800	1
Brückenapotheke	Salicylic acid 50 % (paraffin)	1715Q-07018	1
Hersteller: apomix	Salicylic acid 50 % (paraffin)	6A301111	1
Phoenix (PKH Halle)	Salicylic acid 50 % (paraffin)	2A040313	1
Caelo	Salicylic acid 50 % (paraffin)	13087401	7
Henry Lamotte	Salicylic acid 50 % (paraffin)	5763800	1
Caelo	Salicylic acid 50 % (paraffin)	13160101	5
Caelo	Salicylic acid 50 % (paraffin)	13160102	11
Caelo	Salicylic acid 50 % (paraffin)	13067201	1
Apomix/N/PZN:6639275	Salicylic acid 50 % (paraffin)	9A171213	1
Caelo	Salicylic acid 50 % (paraffin)	12201901	5
Caelo	Salicylic acid 50 % (paraffin)	13087301	8
Apomix	Salicylic acid 50 % (paraffin)	5A250713	1
Caelo	Salicylic acid 50 % (paraffin)	13278601	9
cealo	Salicylic acid 50 % (paraffin)	13278501	3
Caelo	Salicylic acid 50 % (paraffin)	13278501	10
Caelo	Salicylic acid 50 % (paraffin)	13278801	1
Lamotte	Salicylic acid 50 % (paraffin)	5065800	1
Henry Lamotte	Salicylic acid 50 % (paraffin)	5375300	5
Caelo	Salicylic acid 50 % (paraffin)	5375300	1
Caelo	Salicylic acid 50 % (paraffin)	s-100513-1	1

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Supplier	Substance	Batch	Spectra
PKH / 11	Salicylic acid 50 % (paraffin)	2A280116	1
Gehe	Salicylic acid 50 % (paraffin)	14017501	1
Caelo	Salicylic acid 50 % (paraffin)	1401761	1
Caelo	Salicylic acid 50 % (paraffin)	14017601	2
Phönix Gotha	Salicylic acid 50 % (paraffin)	14017601	1
Phoenix 2.07.14	Salicylic acid 50 % (paraffin)	14107901	1
Fagron	Salicylic acid 50 % (paraffin)	14108301	1
Caeo AHDE 25.11.2014	Salicylic acid 50 % (paraffin)	14205101	1
Caelo	Salicylic acid 50 % (paraffin)	14205001	2
Caelo	Salicylic acid 50 % (paraffin)	14337701	2
Caelo	Salicylic acid 50 % (paraffin)	15231701	3
Noweda 26.08.15	Salicylic acid 50 % (paraffin)	15231801	1
Caelo	Salicylic acid 50 % (paraffin)	15247201	4
Caesar&Loretz GmbH	Salicylic acid 50 % (paraffin)	15305901	1
Lamotte	Salicylic acid 50 % (paraffin)	5375300	1
Caelo	Salicylic acid 50 % (paraffin)	15373001	3
Caelo	Salicylic acid 50 % (paraffin)	15372901	2
AHDE08.05.2015	Salicylic acid 50 % (paraffin)	5763800	1
AHD/ Henry Lamotte	Salicylic acid 50 % (paraffin)	5763800	2
Henry Lamotte/Anzag	Salicylic acid 50 % (paraffin)	5448100	1
Henry Lamotte Oils GmbH	Salicylic acid 50 % (paraffin)	5763800	1
Henry Lamotte Olis GmbH...	Salicylic acid 50 % (paraffin)	5763800	1
Henry Lamotte Oils GmbH	Salicylic acid 50 % (paraffin)	5809400	1
noweda / lamotte	Salicylic acid 50 % (paraffin)	5809400	1
Henry Lamotte/Sanacorp	Salicylic acid 50 % (paraffin)	5809400	1
Lamotte	Salicylic acid 50 % (paraffin)	5809400	1
Henry Lamotte/Kehr	Salicylic acid 50 % (paraffin)	5809400	1
AHD/ Henry Lamotte	Salicylic acid 50 % (paraffin)	6001023001	4
Lamotte/Anzag	Salicylic acid 50 % (paraffin)	5809400	1
lamotte	Salicylic acid 50 % (paraffin)	5809400	1
Lamotte/PX	Salicylic acid 50 % (paraffin)	5809400	1
Lamotte/K	Salicylic acid 50 % (paraffin)	6001023001	1
Lamotte	Salicylic acid 50 % (paraffin)	6001023002	3
Henry Lamotte / Sana	Salicylic acid 50 % (paraffin)	5809400	1
Henry Lamotte	Salicylic acid 50 % (paraffin)	5809400	1
Henry Lamotte Olis GmbH...	Salicylic acid 50 % (paraffin)	6001023001	1
Caelo	Salicylic acid 50 % (paraffin)	6001023002	1
Henry Lamotte Oils GmbH	Salicylic acid 50 % (paraffin)	6001862002	1
Noweda	Salicylic acid 50 % (paraffin)	6001023002	1
Apomix / 11	Salicylic acid 50 % (paraffin)	8A240616	1
Caelo	Salicylic acid 50 % (paraffin)	15305601	1
Phoenix	Salicylic acid 50 % (paraffin)	15373101	1
Caelo	Salicylic acid 50 % (paraffin)	16121401	1
Sanacorp, 22.09.2016	Salicylic acid 50 % (paraffin)	16197401	1
Caelo	Salicylic acid 50 % (paraffin)	16121301	1
Caelo	Salicylic acid 50 % (paraffin)	16197401	3
Henry Lamotte / Kehr	Salicylic acid 50 % (paraffin)	6001023002	1
Henry Lamotte Oils GmbH	Salicylic acid 50 % (paraffin)	6001023002	1
Henry Lamotte Olis GmbH...	Salicylic acid 50 % (paraffin)	6001862002	1
Lamotte	Salicylic acid 50 % (paraffin)	6001862002	1
Apomix / 11	Salicylic acid 50 % (paraffin)	4A200613	1
Apomix	Salicylic acid 50 % (paraffin)	1A240113	1
Caelo	Salicylic acid 50 % (paraffin)	613I-01046	1
Fagron	Salicylic acid 50 % (paraffin)	9D28	1
Phönix Gotha	Salicylic acid 50 % (paraffin)	10333901	1
Caelo	Salicylic acid 50 % (paraffin)	11226801	4
Caelo	Salicylic acid 50 % (paraffin)	11274301	1
Caelo	Salicylic acid 50 % (paraffin)	11226601	1
Phönix	Salicylic acid 50 % (paraffin)	11274301	2
Noweda	Salicylic acid 50 % (paraffin)	11333801	1

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Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid 50 % (paraffin)	11333801	7
Caelo	Salicylic acid 50 % (paraffin)	11333602	1
Noweda	Salicylic acid 50 % (paraffin)	11333701	1
Euro OTC	Salicylic acid 50 % (paraffin)	11333801	1
Caelo	Salicylic acid 50 % (paraffin)	12061201	8
Anzag 15.10.12	Salicylic acid 50 % (paraffin)	12201901	1
Noweda	Salicylic acid 50 % (paraffin)	12201901	1
Kehr	Salicylic acid 50 % (paraffin)	12201901	1
Caelo	Salicylic acid 50 % (paraffin)	12061301	1
Phönix, 30.10.2012	Salicylic acid 50 % (paraffin)	12061301	1
Caelo	Salicylic acid 50 % (paraffin)	12228301	11
Gehe	Salicylic acid 50 % (paraffin)	12228301	1
Caelo	Salicylic acid 50 % (paraffin)	12228402	1
Gehe	Salicylic acid 50 % (paraffin)	12305902	1
Caelo	Salicylic acid 50 % (paraffin)	12305901	2
Caelo	Salicylic acid 50 % (paraffin)	12305902	2
Caelo	Salicylic acid 50 % (paraffin)	126061201	1
Sanacorp	Salicylic acid 50 % (paraffin)	1305202	1
Caelo	Salicylic acid 50 % (paraffin)	13052401	4
Phönix Gotha	Salicylic acid 50 % (paraffin)	13052401	1
Caelo	Salicylic acid 50 % (paraffin)	13052502	11
Caelo	Salicylic acid 50 % (paraffin)	13087201	1
Caelo	Salicylic acid 50 % (paraffin)	1309211046	1
Caelo	Salicylic acid 50 % (paraffin)	13160002	1
Caelo	Salicylic acid 50 % (paraffin)	20310812-6	1
Defektur	Salicylic acid 50 % (paraffin)	46/13	1
Caelo	Salicylic acid 50 % (paraffin)	2002311046	1
Caelo	Salicylic acid 50 % (paraffin)	1506211046	1
Gehe	Salicylic acid 50 % (paraffin)	4313M-07018	1
Henry Lamotte	Salicylic acid 50 % (paraffin)	5253300	1
Henry Lamotte/ Anzag	Salicylic acid 50 % (paraffin)	5065800	1
DAC 2005	Salicylic acid 50 % (paraffin)	4960200	1
Phönix	Salicylic acid 50 % (paraffin)	5375300	1
Henry Lamotte/Anzag	Salicylic acid 50 % (paraffin)	5253300	1
Henry Lamotte Oils GmbH	Salicylic acid 50 % (paraffin)	5253300	1
Henry Lamotte	Salicylic acid 50 % (paraffin)	4960200	1
Caelo	Salicylic acid 50 % (paraffin)	AKD2	1

- 58 054 spectra from 332 *Apo-Ident* customers from a total of 19 997 batches from a further 328 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 acid 50 % (paraffin)* 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 acid 50 % (paraffin)* 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	34 024
Type B	0	320	0	63 274
Type C	0	383	4	58 054

The substance/substance group *Salicylic acid 50 % (paraffin)* 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 % (> 99.9689 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.5963 %)	98.9664 % (> 98.1912 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30883	31903	2.04	136.81
30927	31727	6.47	145.48
31727	31727	0.00	142.17
31901	31901	0.00	138.20
31902	31902	0.00	141.99
31903	31903	0.00	137.82
32176	31727	4.75	144.70
32520	32520	0.00	135.08

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Shea butter, refined**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30289-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Shea butter, refined

Special notes

When selecting the *Shea butter, refined* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Shea butter, refined*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Shea butter, ref. . .	13143819	31513	40	1412122
Caelo	Shea butter, ref. . .	14261107	31582	40	20140923
Caelo	Shea butter, ref. . .	15303004	31826	30	20151112
Caelo	Shea butter, ref. . .	15144903	32300	40	20150703

Validation samples

A total of 156379 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 *Shea butter, refined*. These samples are listed above in the [calibration samples](#) section.
- 34194 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 150 spectra of 5 reference samples from the substance/substance group *Shea butter, refined*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Shea butter, refined	10133310	30289	40
Caelo	Shea butter, refined	13143819	31513 [†]	20
Caelo	Shea butter, refined	14261107	31582 [†]	20
Caelo	Shea butter, refined	15303004	31826 [†]	30
Caelo	Shea butter, refined	15144903	32301	40

- 63444 spectra from a total of 1472 batches from further 439 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.

- 59 spectra from 27 *Apo-Ident* customers from 43 batches from the substance/substance group *Shea butter, refined*.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Shea butter, refined	14033304	1
Caelo	Shea butter, refined	14261102	1
Caelo	Shea butter, refined	15144902	1
Caelo	Shea butter, refined	1224210	1
Caelo	Shea butter, refined	10133305	2
Caelo	Shea butter, refined	14033312	2
Abis Pharma/Sanacorp	Shea butter, refined	10-500P/0714	1
Caelo	Shea butter, refined	13143814	1
Caelo	Shea butter, refined	14261108	2
Caelo	Shea butter, refined	13143813	1
Caelo	Shea butter, refined	14033313	1
Caelo	Shea butter, refined	14033314	1
Caelo	Shea butter, refined	14261111	1
Caelo	Shea butter, refined	14261110	1
Sheabutter Import Franz...	Shea butter, refined	14314-18515	1
Sheabutter Import Franz...	Shea butter, refined	14-3-0001	1
Caelo	Shea butter, refined	15303002	2
Caelo	Shea butter, refined	15144907	1
Caelo	Shea butter, refined	15144903	1
Caelo	Shea butter, refined	17031501	1
Caelo	Shea butter, refined	16017204	1
Caelo	Shea butter, refined	16017205	1
ECOCERT/Sanacorp	Shea butter, refined	keine	2
DAC 2006	Shea butter, refined	11346509	1
Gehe	Shea butter, refined	11079802	1
Sheabutter-Import Franz...	Shea butter, refined	1205355	2
Caelo	Shea butter, refined	11346514	1
Caelo	Shea butter, refined	11346509	1
Gehe	Shea butter, refined	11346509	1
Fagron	Shea butter, refined	11J07-N08	1
Fagron	Shea butter, refined	121273	2
Caelo	Shea butter, refined	12242412	1
Caelo	Shea butter, refined	12242404	1
Caelo	Shea butter, refined	12242410	2
Caelo	Shea butter, refined	12242416	2
Fagron	Shea butter, refined	12G12-N14	1
Caelo	Shea butter, refined	12242406	1
Fagron	Shea butter, refined	12g12-n14	1
Fagron	Shea butter, refined	12D16-N03	1
Caesar/Noweda	Shea butter, refined	13143813	1
Caelo	Shea butter, refined	13143810	1
Fagron	Shea butter, refined	13c04-n01	2
Fagron	Shea butter, refined	13C04-N01	4
Franz Thome	Shea butter, refined	400-15	1
Sheabutter-Import Franz...	Shea butter, refined	413-0001	1
Canea/Phönix	Shea butter, refined	SB1351M13	1

- 58 382 spectra from 332 *Apo-Ident* customers from a total of 20 049 batches from a further 328 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 *Shea butter, refined* 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 *Shea butter, refined* 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	34 194
Type B	0	142	8	63 427
Type C	0	43	16	58 377

The substance/substance group *Shea butter, refined* 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 % (> 99.9690 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9711 %)	94.6667 % (> 92.6667 %)
Type C	100.0000 % (> 99.6066 %)	72.8814 % (> 67.7966 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31513	31513	0.00	28.11
31582	31513	7.63	30.82
31826	31513	12.41	32.92
32300	31513	11.14	25.32

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Sodium lactate solution 50%
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30136-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium lactate solution 50%; Natrium lacticum solutum 50%

Special notes

When selecting the *Sodium lactate solution 50%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Sodium lactate solution 50%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium lactate s...	12027310	30621	80	20120131
Caelo	Sodium lactate s...	14039503	31321	40	20140207
Caelo	Sodium lactate s...	16056201	32839	40	AR-17-FG-006366-01

Validation samples

A total of 156379 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 *Sodium lactate solution 50%*. These samples are listed above in the [calibration samples](#) section.
- 34184 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 133 spectra of 4 reference samples from the substance/substance group *Sodium lactate solution 50%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium lactate solution 50%	9258901	30136	20
Caelo	Sodium lactate solution 50%	11024003	30247	33
Caelo	Sodium lactate solution 50%	16056201	32586	40
Caelo	Sodium lactate solution 50%	16056201	32917	40

- 63461 spectra from a total of 1474 batches from further 439 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.

- 365 spectra from 164 *Apo-Ident* customers from 86 batches from the substance/substance group *Sodium lactate solution 50%*.

Supplier	Substance	Batch	Spectra
Caelo	Sodium lactate solution 50%	13111704	10
Caelo	Sodium lactate solution 50%	13111705	5
Caelo	Sodium lactate solution 50%	14039511	2

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Supplier	Substance	Batch	Spectra
Caelo	Sodium lactate solution 50%	14271901	17
Caelo	Sodium lactate solution 50%	13330302	6
Caelo	Sodium lactate solution 50%	14353205	12
Caelo	Sodium lactate solution 50%	15135505	9
Caelo	Sodium lactate solution 50%	14353207	7
Caelo	Sodium lactate solution 50%	15251101	20
Caelo	Sodium lactate solution 50%	16056201	4
Caelo	Sodium lactate solution 50%	15375806	7
Caelo	Sodium lactate solution 50%	12294605	8
Caelo	Sodium lactate solution 50%	13267001	17
Caelo	Sodium lactate solution 50%	11238706	2
Caelo	Sodium lactate solution 50%	12294603	6
Caelo	Sodium lactate solution 50%	13267009	7
Caelo	Sodium lactate solution 50%	13330303	2
Caelo	Sodium lactate solution 50%	3041410	1
Caesar & Lorenz GmbH	Sodium lactate solution 50%	71014/1	1
Caelo	Sodium lactate solution 50%	11024009	5
Caelo	Sodium lactate solution 50%	12294604	6
Caelo	Sodium lactate solution 50%	13267002	2
Caelo	Sodium lactate solution 50%	13267003	9
Caelo	Sodium lactate solution 50%	13330305	7
Caelo	Sodium lactate solution 50%	13330306	1
Caelo	Sodium lactate solution 50%	13330307	7
Fagron	Sodium lactate solution 50%	14/13	1
Caelo	Sodium lactate solution 50%	14039503	12
Euro OTC	Sodium lactate solution 50%	14039503	1
Caelo	Sodium lactate solution 50%	14039507	2
Caelo	Sodium lactate solution 50%	14039508	2
Caelo	Sodium lactate solution 50%	1414Q03157	1
Caelo	Sodium lactate solution 50%	14182902	8
	Sodium lactate solution 50%	14182904	2
Caelo	Sodium lactate solution 50%	14182904	5
Caelo	Sodium lactate solution 50%	14182903	2
phoenix	Sodium lactate solution 50%	14271901	1
Phönix	Sodium lactate solution 50%	14271901	1
Caelo	Sodium lactate solution 50%	14271902	2
Caelo	Sodium lactate solution 50%	14271904	7
Caelo	Sodium lactate solution 50%	14271906	2
Caelo	Sodium lactate solution 50%	14271903	1
Caelo	Sodium lactate solution 50%	14271907	6
Euro OTC	Sodium lactate solution 50%	14271907	1
Gehe 12.1.15	Sodium lactate solution 50%	14271907	1
Fagron	Sodium lactate solution 50%	14271907	1
Caelo	Sodium lactate solution 50%	14271908	2
Caelo	Sodium lactate solution 50%	14353204	2
Caelo	Sodium lactate solution 50%	14353201	2
Caelo	Sodium lactate solution 50%	14353202	2
Alliance health	Sodium lactate solution 50%	14353205	1
Noweda 18.05.2015	Sodium lactate solution 50%	14353205	1
Caesar & Loretz GmbH	Sodium lactate solution 50%	14353205	1
Caelo	Sodium lactate solution 50%	14353208	1
Caelo	Sodium lactate solution 50%	14353210	7
Phoenix	Sodium lactate solution 50%	14353210	1
Fagron	Sodium lactate solution 50%	14A21-B10	1
Fagron	Sodium lactate solution 50%	14A21-810-295977	1
Fagron	Sodium lactate solution 50%	14A21-B10-290492	2
Caelo	Sodium lactate solution 50%	14A21-B10-295977	1
Fagron	Sodium lactate solution 50%	14a21-b10-295977	1
Caelo	Sodium lactate solution 50%	15135508	2
Caelo	Sodium lactate solution 50%	1525110	1

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Supplier	Substance	Batch	Spectra
Phoenix	Sodium lactate solution 50%	15251101	1
Caelo	Sodium lactate solution 50%	15251102	4
Caesar & Loretz/Sanacorp	Sodium lactate solution 50%	15251101	1
Caelo	Sodium lactate solution 50%	15375805	1
Caelo	Sodium lactate solution 50%	15375808	4
Caesar & Loretz/Noweda	Sodium lactate solution 50%	15375806	1
Caesar&Loretz GmbH	Sodium lactate solution 50%	15375806	1
Phoenix	Sodium lactate solution 50%	16056201	1
Ebert 02.08.2016	Sodium lactate solution 50%	15375808	1
Caelo	Sodium lactate solution 50%	16056206	4
Caelo	Sodium lactate solution 50%	2014U-03157	1
Caelo	Sodium lactate solution 50%	507213157	1
Caelo	Sodium lactate solution 50%	11238701	4
Caelo	Sodium lactate solution 50%	11024001	1
Caelo	Sodium lactate solution 50%	11063006	1
Caelo	Sodium lactate solution 50%	11238707	2
Caelo	Sodium lactate solution 50%	11238712	2
Caelo	Sodium lactate solution 50%	12027301	1
Gehe	Sodium lactate solution 50%	11238712	1
Caelo	Sodium lactate solution 50%	12027303	3
Caelo	Sodium lactate solution 50%	12027310	3
phönix, 30.08.2012	Sodium lactate solution 50%	12027312	1
Caelo	Sodium lactate solution 50%	12180404	5
Caelo	Sodium lactate solution 50%	12180406	2
phönix	Sodium lactate solution 50%	12180404/8	1
Beiersdorf AG / Noweda	Sodium lactate solution 50%	12180406	1
Caelo	Sodium lactate solution 50%	12180407	5
Caelo	Sodium lactate solution 50%	1218407	1
Caelo	Sodium lactate solution 50%	12180408	2
Phönix	Sodium lactate solution 50%	12180407	1
Sanacorp	Sodium lactate solution 50%	12180407	1
Anzag 27.02.2013	Sodium lactate solution 50%	12294603	1
Gehe	Sodium lactate solution 50%	12294603	1
Kehr	Sodium lactate solution 50%	12294604	1
Noweda	Sodium lactate solution 50%	12294604	2
Caelo	Sodium lactate solution 50%	12294607	6
Caelo	Sodium lactate solution 50%	12294610	4
Fagron	Sodium lactate solution 50%	12J18-M04	5
Phönix, 20.09.2013	Sodium lactate solution 50%	13111705	1
Bergchemie	Sodium lactate solution 50%	13111704	1
Caelo	Sodium lactate solution 50%	13267005	1
Caelo	Sodium lactate solution 50%	13267006	2
Gehe	Sodium lactate solution 50%	13267009	1
Caelo	Sodium lactate solution 50%	13330304	2
gehe	Sodium lactate solution 50%	13330302	1
Caelo	Sodium lactate solution 50%	14011301	1
Sanacorp	Sodium lactate solution 50%	14039508	1
Caesar&lorenz,Phoenix	Sodium lactate solution 50%	14182902	1
Caelo	Sodium lactate solution 50%		1
phönix	Sodium lactate solution 50%	9/AKD56	1
Caelo	Sodium lactate solution 50%	20310511-1	1
Caelo	Sodium lactate solution 50%	3111Q-03157	1
Phönix Gotha	Sodium lactate solution 50%	K40875122	1
Caelo	Sodium lactate solution 50%	N-260313-3	1

- 58 076 spectra from 331 *Apo-Ident* customers from a total of 20 007 batches from a further 328 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

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

Validation results

The validation runs checked whether the substance/substance group *Sodium lactate solution 50%* 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 *Sodium lactate solution 50%* 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	34 184
Type B	0	129	4	63 461
Type C	0	347	18	58 076

The substance/substance group *Sodium lactate solution 50%* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	96.9925 % (> 94.7368 %)
Type C	100.0000 % (> 99.5963 %)	95.0685 % (> 94.2466 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30621	32839	2.99	36.16
31321	32839	2.19	38.02
32839	32839	0.00	36.58

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Sodium lactate solution 60%
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30525-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium lactate solution 60%; Natrium lacticum solutum 60%

Special notes

When selecting the *Sodium lactate solution 60%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Sodium lactate solution 60%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Sodium lactate s...	1201037-01	30525	40	1507187
Euro OTC	Sodium lactate s...	1201037-01	31703	40	20120224
Euro OTC	Sodium lactate s...	1310007-01	31821	40	20140217
Euro OTC	Sodium lactate s...	1310007-01	32813	40	20140217

Validation samples

A total of 156 379 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 *Sodium lactate solution 60%*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 64 spectra of 3 reference samples from the substance/substance group *Sodium lactate solution 60%*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sodium lactate solution 60%	1201037-01	31703 [†]	20
Euro OTC	Sodium lactate solution 60%	1310007-01	31821 [†]	20
Euro OTC	Sodium lactate solution 60%	1310007-01	not required	24

- 63 530 spectra from a total of 1475 batches from further 439 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 *Sodium lactate solution 60%*.

Supplier	Substance	Batch	Spectra
Euro OTC	Sodium lactate solution 60%	1310007-01	1

[†]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*.

- 58 440 spectra from 332 *Apo-Ident* customers from a total of 20 091 batches from a further 328 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 *Sodium lactate solution 60%* 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 *Sodium lactate solution 60%* 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	34 184
Type B	0	64	0	63 530
Type C	0	1	0	58 440

The substance/substance group *Sodium lactate solution 60%* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.6250 %)
Type C	100.0000 % (> 99.6053 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30525	30525	0.00	56.09
31703	30525	4.34	58.14
31821	30525	11.41	59.96
32813	30525	17.10	62.54

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Sodium laureth sulfate solution 27%
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30936-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium laureth sulfate solution 27%; Natrii laurylethersulfatis solutio 27 %; Sodium laureth sulphate solution 27%; Solutio natrii laurylaethersulfurici 27 %

Special notes

When selecting the *Sodium laureth sulfate solution 27%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Sodium laureth sulfate solution 27%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium laureth s...	12315211	30936	50	20121029
Caelo	Sodium laureth s...	13069915	31114	39	20130402
Caelo	Sodium laureth s...	14049902	31349	40	8930
Caelo	Sodium laureth s...	161968	32696	30	20161010*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 159 spectra of 4 reference samples from the substance/substance group *Sodium laureth sulfate solution 27%*. These samples are listed above in the [calibration samples](#) section.
- 34 185 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 150 spectra of 5 reference samples from the substance/substance group *Sodium laureth sulfate solution 27%*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium laureth sulfate solut...	10372703	30345	40
Caelo	Sodium laureth sulfate solut...	14049902	31349 [†]	20
Caelo	Sodium laureth sulfate solut...	161968	32696 [†]	10
Caelo	Sodium laureth sulfate solut...	16196801	32818	40
Caelo	Sodium laureth sulfate solut...	163071	33090	40

- 63 444 spectra from a total of 1472 batches from further 439 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.

*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.

[†]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*.

- 35 spectra from 15 *Apo-Ident* customers from 24 batches from the substance/substance group *Sodium laureth sulfate solution 27%*.

Supplier	Substance	Batch	Spectra
Caelo	Sodium laureth sulfate solut...	12341104	1
Caelo	Sodium laureth sulfate solut...	13241101	1
Caelo	Sodium laureth sulfate solut...	14197915	3
Caesar & Loretz GmbH Hi...	Sodium laureth sulfate solut...	14049913	1
Caelo	Sodium laureth sulfate solut...	14355314	4
Caelo	Sodium laureth sulfate solut...	15145017	2
Caelo	Sodium laureth sulfate solut...	15145010	1
Sanacorp	Sodium laureth sulfate solut...	14049902	1
Caelo	Sodium laureth sulfate solut...	13241004	1
Caelo	Sodium laureth sulfate solut...	14049902	1
Caelo	Sodium laureth sulfate solut...	14049904	1
Caelo	Sodium laureth sulfate solut...	14355315	1
Caelo	Sodium laureth sulfate solut...	14197920	1
Caelo	Sodium laureth sulfate solut...	15145004	1
Caelo	Sodium laureth sulfate solut...	14355310	1
Caelo	Sodium laureth sulfate solut...	12315203	1
Caelo	Sodium laureth sulfate solut...	12044308	4
Caesar & Loretz GmbH, 4...	Sodium laureth sulfate solut...	12315211	1
Caelo	Sodium laureth sulfate solut...	12044307	1
Caelo	Sodium laureth sulfate solut...	12315211	1
Caelo	Sodium laureth sulfate solut...	13069903	1
Caelo	Sodium laureth sulfate solut...	13069905	1
Caelo	Sodium laureth sulfate solut...	13241001	1
Caelo	Sodium laureth sulfate solut...	13069911	1
Caelo	Sodium laureth sulfate solut...	2613M-01907	1
Caelo	Sodium laureth sulfate solut...	14197916	1

- 58 406 spectra from 332 *Apo-Ident* customers from a total of 20 068 batches from a further 328 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 *Sodium laureth sulfate solution 27%* 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 *Sodium laureth sulfate solution 27%* 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	159	0	34 185
Type B	0	133	17	63 444
Type C	0	35	0	58 406

The substance/substance group *Sodium laureth sulfate solution 27%* 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 % (> 99.9690 %)	100.0000 % (> 96.2264 %)
Type B	100.0000 % (> 99.9710 %)	88.6667 % (> 86.6667 %)
Type C	100.0000 % (> 99.5965 %)	100.0000 % (> 82.8571 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30936	31349	3.87	29.01
31114	31349	4.67	27.71
31349	31349	0.00	25.09
32696	32696	0.00	22.10

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Soft ointment**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30896-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Soft ointment; Unguentum molle

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Soft ointment*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Soft ointment	12353301	30896	80	20121218
Henry Lamotte	Soft ointment	5215100	30924	50	20111111
Caelo	Soft ointment	14080501	31452	40	AR-15-FG-000142-01
Caelo	Soft ointment	153768	31984	40	20151103*
Caelo	Soft ointment	160833	32097	40	20160322*
Caelo	Soft ointment	163134	32871	40	20161116*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 290 spectra of 6 reference samples from the substance/substance group *Soft ointment*. These samples are listed above in the [calibration samples](#) section.
- 34 054 spectra from a total of 792 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 750 spectra of 17 reference samples from the substance/substance group *Soft ointment*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Soft ointment	10377401	30291	40
Caelo	Soft ointment	12353301	30882	40
Caelo	Soft ointment	153768	31983	60
Caelo	Soft ointment	153768	31984 [†]	20
Caelo	Soft ointment	153770	31985	60
Caelo	Soft ointment	153770	31986	60
Caelo	Soft ointment	153772	31987	60
Caelo	Soft ointment	153772	31988	60
Caelo	Soft ointment	160830	32094	40
Caelo	Soft ointment	160831	32095	30
Caelo	Soft ointment	160832	32096	40
Caelo	Soft ointment	161463	32406	40
Caelo	Soft ointment	161464	32407	40
Caelo	Soft ointment	162452	32496	40
Caelo	Soft ointment	162453	32497	40
Caelo	Soft ointment	162454	32498	40
Caelo	Soft ointment	162455	32499	40

*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.

[†]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*.

- 62 844 spectra from a total of 1463 batches from further 439 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.

- 876 spectra from 221 *Apo-Ident* customers from 204 batches from the substance/substance group *Soft ointment*.

Supplier	Substance	Batch	Spectra
Caelo	Soft ointment	1097697	2
Caelo	Soft ointment	14007301	19
Caelo	Soft ointment	14007501	10
Caelo	Soft ointment	14202001	7
Caelo	Soft ointment	14202301	25
Caelo	Soft ointment	14202302	7
Caelo	Soft ointment	14375602	18
Caelo	Soft ointment	14375801	5
Caelo	Soft ointment	14375601	8
Caelo	Soft ointment	14375901	5
Caelo	Soft ointment	15059301	9
Caelo	Soft ointment	15204401	19
Caelo	Soft ointment	15204501	16
Caelo	Soft ointment	15377101	21
Caelo	Soft ointment	16083301	3
Caelo	Soft ointment	16083101	9
Caelo	Soft ointment	16083001	12
Caelo	Soft ointment	16083002	11
Bombastus	Soft ointment	284057	1
Henry Lamotte Oils	Soft ointment	5600500	3
HENRY LAMOTTE OILS GmbH	Soft ointment	6001368015	2
Anzag	Soft ointment	269470	1
Anzag	Soft ointment	267553	1
Caelo	Soft ointment	12353401	10
Caelo	Soft ointment	11282101	3
Caelo	Soft ointment	13192501	23
Caelo	Soft ointment	13192601	26
Caelo	Soft ointment	13192502	3
Caelo	Soft ointment	13375402	10
Bombastus	Soft ointment	278047	1
Caelo	Soft ointment	13192701	5
Lamotte	Soft ointment	5375800	1
Caelo	Soft ointment	13375501	10
Bombastus	Soft ointment	275422	4
Caelo	Soft ointment	5011504	1
Caelo	Soft ointment	5081405	1
caesar&loretz GmbH,Phönix	Soft ointment	12194502	2
Caelo	Soft ointment	7051510	1
Caelo	Soft ointment	1097763	1
Gehe/04.12.14	Soft ointment	12353301	1
Caelo	Soft ointment	13053801	17
Caelo	Soft ointment	1314I-02542	1
Caelo	Soft ointment	1314I2542	1
Gehe am 25.02.14	Soft ointment	13375402	1
Caelo	Soft ointment	13375503	2

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Supplier	Substance	Batch	Spectra
Caelo	Soft ointment	13387402	16
Berkel AHK	Soft ointment	13387402	1
Phoenix	Soft ointment	13387403	1
Caelo	Soft ointment	13E13-T12-003670	1
Fagron	Soft ointment	13I24-T01-006925	2
Euro OTC	Soft ointment	13E13-T13-003675	1
Fagron	Soft ointment	13I24-T02-006930	1
Fagron	Soft ointment	13I24-T03-006933	1
Fagron	Soft ointment	13I24-T04-006936	1
Fagron	Soft ointment	13I24-T01-006925	1
PHOENIX 10.03.2014	Soft ointment	14007302	1
Caelo	Soft ointment	14007302	2
Caelo	Soft ointment	14007402	2
Caelo	Soft ointment	14007601	22
Noweda	Soft ointment	14007601	1
Berkel AHK	Soft ointment	14007601	1
Caelo	Soft ointment	14080101	1
Caelo	Soft ointment	14080201	11
Alliance Healthcare	Soft ointment	14080201	1
Euro OTC	Soft ointment	14080201	1
Caelo	Soft ointment	14080301	2
Sanacorp	Soft ointment	14080301	1
Caelo	Soft ointment	14080501	7
Caesar &Loretz GmbH	Soft ointment	14080501	1
Caesar & Loretz	Soft ointment	14080501	1
Caelo	Soft ointment	14201801	2
Caelo	Soft ointment	14201901	6
Fagron	Soft ointment	14201901	1
Berkel AHK	Soft ointment	14202001	1
Caelo	Soft ointment	14202201	13
Caelo	Soft ointment	14202011	1
Berkel AHK	Soft ointment	14202201	2
Gehe	Soft ointment	14202301	2
Fagron	Soft ointment	14202301	1
Allianc 03.02.15	Soft ointment	14375601	1
Caelo	Soft ointment	14205001	1
Phönix	Soft ointment	14375601	1
Caelo	Soft ointment	1422001	1
Caesar&Loretz GmbH/Sana...	Soft ointment	14375602	1
AHDE 03.06.2015	Soft ointment	14375602	2
Allianz Healthcare 11.0...	Soft ointment	14375602	1
Caelo	Soft ointment	14375603	1
Sanacorp	Soft ointment	14375801	1
Caelo	Soft ointment	1437591	1
Fagron	Soft ointment	14E16-T03-012547	1
Fagron	Soft ointment	14e16-t03-012548	1
Fagron	Soft ointment	14E16-T03-012548	1
Caelo	Soft ointment	15059401	4
Caelo	Soft ointment	15059402	2
Caelo	Soft ointment	15059501	1
Caelo	Soft ointment	15059601	3
Caelo	Soft ointment	15204402	1
Caelo	Soft ointment	15204602	4
Caelo	Soft ointment	15204701	2
Caelo	Soft ointment	15376801	10
Sanacorp	Soft ointment	15376801	1
Noweda	Soft ointment	15376901	2
Caelo	Soft ointment	15376901	5
Caelo	Soft ointment	15377001	6
InfectoPharm/Noweda	Soft ointment	15377001	1

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Supplier	Substance	Batch	Spectra
Noweda	Soft ointment	15377001	1
Bombastus	Soft ointment	15377001	1
caesar&loretz GmbH,Phönix	Soft ointment	15959301	1
Fargron/ Noweda	Soft ointment	15A30-T02-018955	2
Fargron	Soft ointment	15A30	1
Fargron	Soft ointment	15A30-T02-018955	2
Fargron	Soft ointment	15F24-T16-023904	4
Fargron	Soft ointment	15F24T16023904	1
Fargron	Soft ointment	15f24-t16-023904	1
Caelo	Soft ointment	16024401	1
Phoenix	Soft ointment	16083002	1
Wolf-Apotheke	Soft ointment	16083101	1
Bombastus	Soft ointment	16083101	1
Euro OTC	Soft ointment	16083101	1
Ebert & Jacobi 19.07...	Soft ointment	16083101	1
Caelo	Soft ointment	16146201	2
Caelo	Soft ointment	16146301	3
Caelo	Soft ointment	16146401	3
Caelo	Soft ointment	16146502	5
Caelo	Soft ointment	16245201	2
Caesar & Loretz	Soft ointment	16245201	1
Caelo	Soft ointment	16245301	2
Caelo	Soft ointment	16245401	1
Caelo	Soft ointment	16A21T05029597	1
Fargron	Soft ointment	16A21-T05-029597	2
Caelo	Soft ointment	23061403	1
Fargron	Soft ointment	2514M-02542	1
Bombastus	Soft ointment	281897	1
Phönix Gotha	Soft ointment	286010	1
Bombastus	Soft ointment	286012	6
Bombastus	Soft ointment	288013	2
Bombastus	Soft ointment	288704	1
Phönix Gotha	Soft ointment	291331	1
Bomastus	Soft ointment	291333	1
Bombastus	Soft ointment	291333	3
Bombastus	Soft ointment	293336	1
Bombastus	Soft ointment	295313	1
Bombastus	Soft ointment	297077	6
Bombastus	Soft ointment	302327	2
Caelo	Soft ointment	31031503	1
Henry Lamotte oils GmbH...	Soft ointment	5448300	1
Caelo	Soft ointment	51123/1Sie	1
Henry Lamotte Oils GmbH...	Soft ointment	5448300	1
Henry Lamotte oils GmbH...	Soft ointment	5691000	1
ahd/lamotte	Soft ointment	5789000	1
Henry Lamotte Olis GmbH...	Soft ointment	5789000	3
Lamotte	Soft ointment	5789000	1
Henry Lamotte/Anzag	Soft ointment	6001368001	1
Henry Lamotte Olis GmbH...	Soft ointment	6001368015	2
Henry Lamotte/Anzag	Soft ointment	6001368015	1
Bombastus	Soft ointment	6862381	1
Sanacorp	Soft ointment	94/AKD1	1
Sanacorp	Soft ointment	96/AKD3	1
Sanacorp	Soft ointment	97/AKD4	1
Caelo	Soft ointment	Caelo	1
Caelo	Soft ointment		1
Phönix Gotha	Soft ointment	261107	1
Phönix Gotha	Soft ointment	268872	1
Bombastus	Soft ointment	269469	1
Bombastus	Soft ointment	269468	1

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Supplier	Substance	Batch	Spectra
Bombastus	Soft ointment	262274	1
Phönix Gotha	Soft ointment	271425	1
Bombastus	Soft ointment	271430	1
Caelo	Soft ointment	612212542	1
Caelo	Soft ointment	7071202	1
Caelo	Soft ointment	11132901	1
Caelo	Soft ointment	10111201	1
Caelo	Soft ointment	11133001	2
Noweda	Soft ointment	11133001	1
Caelo	Soft ointment	11133002	1
Caelo	Soft ointment	11256301	1
Phönix	Soft ointment	11256301	1
Caelo	Soft ointment	11256302	1
Caelo	Soft ointment	11256701	5
Noweda	Soft ointment	11256701	1
Caelo	Soft ointment	11282102	2
Caelo	Soft ointment	11282201	7
Noweda	Soft ointment	11282201	1
Caelo	Soft ointment	11282301	2
Caelo	Soft ointment	118282301	1
Caelo	Soft ointment	12045104	1
Caelo	Soft ointment	12045401	1
Caesar&lorenz,Phoenix	Soft ointment	12045401	1
Caesar&lorenz,Phoenix	Soft ointment	12045501	1
Caelo	Soft ointment	12045501	3
Caelo	Soft ointment	12045601	1
Caelo	Soft ointment	12045701	5
Phoenix	Soft ointment	12045701	1
Hustadt Apotheke	Soft ointment	12045701	1
Caelo	Soft ointment	12045702	5
Caelo	Soft ointment	120502/6	1
Caelo	Soft ointment	12091303	2
Caelo	Soft ointment	12091401	5
Caesar&lorenz,Phoenix	Soft ointment	12091303	1
Anzag ek:5,12EUR 19.09.12	Soft ointment	12091402	1
Gehe	Soft ointment	12091401	1
Noweda	Soft ointment	12091402	1
Caelo	Soft ointment	12091402	6
Caelo	Soft ointment	12091403	1
Caelo	Soft ointment	12194401	3
Caelo	Soft ointment	12194501	5
Gehe	Soft ointment	12194501	2
Sanacorp	Soft ointment	12194501	1
Caelo	Soft ointment	12194502	3
Caelo	Soft ointment	12194601	12
Noweda	Soft ointment	12194601	1
Phönix	Soft ointment	12194601	1
Caelo	Soft ointment	12194701	2
phönix	Soft ointment	12194701	1
Caelo	Soft ointment	12353201	15
Großhandel	Soft ointment	12353201	1
Noweda	Soft ointment	12353201	1
Anzag 31.01.13 ek: 5,10EUR	Soft ointment	12353201	1
Caelo	Soft ointment	12353301	9
Anzag 23.01.2013	Soft ointment	12353301	1
fargon/Sanacorp	Soft ointment	12353301	1
Bombastus	Soft ointment	12353301	1
Caelo	Soft ointment	12353302	1
Caelo	Soft ointment	1294502	1
Caelo	Soft ointment	1253201	1

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Supplier	Substance	Batch	Spectra
Fagron	Soft ointment	12e23-t01	1
Caelo	Soft ointment	130221/1	1
Fagron	Soft ointment	12G09-T02	1
Fagron	Soft ointment	12E23-T01	1
Caelo	Soft ointment	13053601	15
Kehr	Soft ointment	13053601	1
Caesar & Loretz GmbH, 4...	Soft ointment	13053601	1
Gehe	Soft ointment	13053601	1
Caelo	Soft ointment	13053602	5
Caelo	Soft ointment	13053701	1
Phönix	Soft ointment	13053801	1
Großhandel	Soft ointment	13053801	1
20; 27.08.13	Soft ointment	13053801	1
Caelo	Soft ointment	13053901	6
Caelo	Soft ointment	1319201	1
Gehe 10.10.13	Soft ointment	13192601	1
Phoenix	Soft ointment	13192601	1
gehe 04.12.13	Soft ointment	13192601	1
Sanacorp	Soft ointment	13192701	1
Caelo	Soft ointment	13192801	2
Caelo	Soft ointment	13192901	14
Sanacorp	Soft ointment	13192901	1
Phönix	Soft ointment	13192901	1
Caelo	Soft ointment	13192902	3
Euro OTC	Soft ointment	13192902	1
Sanacorp	Soft ointment	13375402	1
Fagron	Soft ointment	13387402	1
Gehe am 04.02.2014	Soft ointment	13387402	1
Caelo	Soft ointment	13387403	4
Fagron	Soft ointment	13A08-T12-000186	1
Fagron	Soft ointment	13A08-T13-000189	1
Fagron	Soft ointment	13C04-T04-0002	1
Fagron	Soft ointment	13C04-T04-001709	3
Fagron	Soft ointment	13C04-T04-001710	3
Fagron	Soft ointment	13C04-T05	2
Fagron	Soft ointment	13E13-T12-003669	1
Fagron	Soft ointment	13E13-T12-003670	2
Fagron	Soft ointment	13E13-T14-003679	2
Phoenix	Soft ointment	14007601	1
Phönix	Soft ointment	14201801	1
Caelo	Soft ointment	18121206	1
Caelo	Soft ointment	2513A-02542	1
Caelo	Soft ointment	1912A-02542	1
Caelo	Soft ointment	20230712-4	1
Bombastus	Soft ointment	275424	1
Bombastus	Soft ointment	276854	1
Bombastus	Soft ointment	278048	2
Phönix Gotha	Soft ointment	278046	1
Bombastus	Soft ointment	280166	2
Alliance Healthcare/Hed...	Soft ointment	281897	2
Caelo	Soft ointment	284057	1
Fagron	Soft ointment	4113A-02542	1
Caelo	Soft ointment	3213E2542	1
Henry Lamotte,Phönix	Soft ointment	5067500	1
H. Lamotte	Soft ointment	5067500	1
Henry Lamotte	Soft ointment	5067500	1
Henry Lamotte,Anzag	Soft ointment	5189900	2
HenryLamotte/Phoenix	Soft ointment	5189900	1
Lamotte	Soft ointment	5215100	1
Henry Lamotte/GEHE	Soft ointment	5215100	1

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Supplier	Substance	Batch	Spectra
Henry Lam./ Sanacorp	Soft ointment	5215100	1
Finze	Soft ointment	5215100	1
lamotte/Noweda	Soft ointment	5265300	2
lamotte7anzag	Soft ointment	5294600	1
Henry Lamotte/GEHE	Soft ointment	5317100	1
Henry Lamotte Oils	Soft ointment	5317100	1
Fiebig 32.01.13 ek:4,84EUR	Soft ointment	5317100	1
Henry Lamotte	Soft ointment	5317100	1
H. Lamotte	Soft ointment	5317100	1
H.Lamotte / Anzag	Soft ointment	5317100	1
Henry Lamotte oils GmbH	Soft ointment	5321600	2
Henra Lamotte	Soft ointment	5321600	1
Henry Lamotte/GEHE	Soft ointment	5375800	1
Lamotte/ Anzag	Soft ointment	5375800	1
Gehe	Soft ointment	5375800	1
Henry Lamotte/Anzag	Soft ointment	5448300	1
Henry Lamotte Oils GMBH	Soft ointment	5496100	1
Lamotte/ Anzag	Soft ointment	5496100	1
Henry Lamotte Oils GmbH...	Soft ointment	5496100	2
Henry Lamotte Oils GmbH	Soft ointment	5496100	1
Lamotte/Krieger/20.05.2...	Soft ointment	5496100	1
Noweda	Soft ointment	60089901	1
Henry Lamotte Oils/ Gehe	Soft ointment	61580	1
Caelo	Soft ointment	92810389	1
Caelo	Soft ointment	I3192502	1

- 57 565 spectra from 332 *Apo-Ident* customers from a total of 19 891 batches from a further 328 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 *Soft 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 *Soft 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	290	0	34 054
Type B	0	722	28	62 844
Type C	0	830	46	57 565

The substance/substance group *Soft 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 % (> 99.9689 %)	100.0000 % (> 97.9310 %)
Type B	100.0000 % (> 99.9710 %)	96.2667 % (> 95.8667 %)
Type C	100.0000 % (> 99.5963 %)	94.7489 % (> 94.4064 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30896	31984	5.43	105.31
30924	31984	10.40	117.45
31452	31452	0.00	91.57
31984	31984	0.00	102.70
32097	32097	0.00	90.72
32871	32871	0.00	99.85

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Softisan® 378**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30887-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Softisan® 378; Adeps solidus 378

Special notes

When selecting the *Softisan® 378* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Softisan® 378*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Softisan® 378	12K27-N05	30887	60	20121204
Fagron	Softisan® 378	13D26-N12	31117	40	1407632
Caelo	Softisan® 378	13370104	31472	40	20131119
Caelo	Softisan® 378	14301114	32298	30	20141118
Fagron	Softisan® 378	15G20-B10-326361	32964	40	1704407

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 210 spectra of 5 reference samples from the substance/substance group *Softisan*[®] 378. These samples are listed above in the [calibration samples](#) section.
- 34 134 spectra from a total of 793 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 170 spectra of 5 reference samples from the substance/substance group *Softisan*[®] 378.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	<i>Softisan</i> [®] 378	10F09-N12	30295	40
Caelo	<i>Softisan</i> [®] 378	14301114	32298 [†]	10
Caelo	<i>Softisan</i> [®] 378	14301114	32299	40
Caelo	<i>Softisan</i> [®] 378	162686	33078	40
Caelo	<i>Softisan</i> [®] 378	162686	33101	40

- 63 424 spectra from a total of 1474 batches from further 439 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.

- 81 spectra from 29 *Apo-Ident* customers from 49 batches from the substance/substance group *Softisan*[®] 378.

[†]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*.

Supplier	Substance	Batch	Spectra
Sino Phyto	Softisan [®] 378	2012060444	1
Caelo	Softisan [®] 378	18011302	1
Caelo	Softisan [®] 378	14301104	2
Fagron	Softisan [®] 378	514E-02911	1
Caelo	Softisan [®] 378	13370104	3
Fagron	Softisan [®] 378	14F11-B04	3
Caelo	Softisan [®] 378	14301113	1
Caelo	Softisan [®] 378	15G20-B10-316518	2
Caelo	Softisan [®] 378	15G20B10320309	1
Caelo	Softisan [®] 378	15gb10326361	1
Bionorica/Gehe	Softisan [®] 378	75850	3
Caelo	Softisan [®] 378	16010402	1
THC Pharma	Softisan [®] 378	2013091014	2
Gehe Kassel 09.02.2015	Softisan [®] 378	75850	1
Caelo	Softisan [®] 378	1081408	1
Caelo	Softisan [®] 378	4041501	1
Fagron	Softisan [®] 378	13H22-N01	3
Caelo	Softisan [®] 378	13370102	2
Fagron	Softisan [®] 378	12I24-N01	1
Fagron	Softisan [®] 378	13D26-N12	10
Caelo	Softisan [®] 378	13370112	1
Thc	Softisan [®] 378	2012060444	1
Caelo	Softisan [®] 378	16021507	1
Alliance Health.14.08.2...	Softisan [®] 378		1
Caelo	Softisan [®] 378	73059	1
Fagron	Softisan [®] 378	11520	2
Caelo	Softisan [®] 378	28031401	1
Caelo	Softisan [®] 378	57657	1
Caelo	Softisan [®] 378	11121304	1
Sanacorp	Softisan [®] 378	3/AKD1	1
Caelo	Softisan [®] 378	3071201	1
Caelo	Softisan [®] 378	10310008	1
Caelo	Softisan [®] 378	10310003	1
Caelo	Softisan [®] 378	11359302	1
Fagron	Softisan [®] 378	12/24-N01	1
Caelo	Softisan [®] 378	13012707	4
Caelo	Softisan [®] 378	13012703	1
Gehe	Softisan [®] 378	12D02-N07	1
Fagron	Softisan [®] 378	13B11-N01	1
Caelo	Softisan [®] 378	13012704	1
Fagron	Softisan [®] 378	13D26-N02	1
Fagron	Softisan [®] 378	13H22-N01	1
Caelo	Softisan [®] 378	14111312	1
Caelo	Softisan [®] 378	14301103	2
Noweda	Softisan [®] 378	2012060444	1
Caelo	Softisan [®] 378	14301112	1
THC Pharma	Softisan [®] 378		1
Fagron	Softisan [®] 378	209602	3
Caelo	Softisan [®] 378	21031310	1
Fagron	Softisan [®] 378	303624	1
Caelo	Softisan [®] 378	27091306	1
Fagron	Softisan [®] 378	011520	1
Caelo	Softisan [®] 378	209602	1

- 58 360 spectra from 332 *Apo-Ident* customers from a total of 20 043 batches from a further 328 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 *Softisan*® 378 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 *Softisan*® 378 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	210	0	34 134
Type B	0	167	3	63 336
Type C	0	60	21	58 354

The substance/substance group *Softisan*® 378 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 % (> 99.9690 %)	100.0000 % (> 97.1429 %)
Type B	100.0000 % (> 99.9712 %)	98.2353 % (> 96.4706 %)
Type C	100.0000 % (> 99.5973 %)	74.0741 % (> 70.3704 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30887	31117	7.68	14.47
31117	31117	0.00	13.12
31472	31117	3.87	12.70
32298	31117	0.71	13.20
32964	32964	0.00	16.08

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Sorbitan- and glycerol monooleate**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31574-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sorbitan- and glycerol monooleate

Special notes

When selecting the *Sorbitan- and glycerol monooleate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Sorbitan- and glycerol monooleate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sorbitan- and gl...	14202402	31574	40	AR-15-FG-009320-01
Caelo	Sorbitan- and gl...	15122301	31726	40	20150420

Validation samples

A total of 156379 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 *Sorbitan- and glycerol monooleate*. These samples are listed above in the [calibration samples](#) section.
- 34264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 52 spectra of 3 reference samples from the substance/substance group *Sorbitan- and glycerol monooleate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sorbitan- and glycerol monoo...	14202402	31574 [†]	20
Caelo	Sorbitan- and glycerol monoo...	15122301	31726 [†]	20
Caelo	Sorbitan- and glycerol monoo...	16234301	not required	12

- 63542 spectra from a total of 1474 batches from further 439 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 *Sorbitan- and glycerol monooleate*.
- 58441 spectra from 332 *Apo-Ident* customers from a total of 20092 batches from a further 329 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](#),

[†]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 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 *Sorbitan- and glycerol monooleate* 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 *Sorbitan- and glycerol monooleate* 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	34 264
Type B	0	52	0	63 542
Type C	0	0	0	58 441

The substance/substance group *Sorbitan- and glycerol monooleate* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 88.4615 %)
Type C	100.0000 % (> 99.5963 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31574	31574	0.00	32.65
31726	31574	7.24	34.99

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Sorbitan trioleate**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31031-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Sorbitan trioleate; Sorbitani trioleas

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Sorbitan trioleate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sorbitan trioleate	12171410	31031	39	1407273
Caelo	Sorbitan trioleate	13317202	31130	40	20131017
Caelo	Sorbitan trioleate	13317212	31459	40	20131017

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 119 spectra of 3 reference samples from the substance/substance group *Sorbitan trioleate*. These samples are listed above in the [calibration samples](#) section.
- 34 225 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 37 spectra of 2 reference samples from the substance/substance group *Sorbitan trioleate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sorbitan trioleate	10109108	30316	17
Caelo	Sorbitan trioleate	13317212	31459 [†]	20

- 63 557 spectra from a total of 1475 batches from further 439 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.

- 24 spectra from 14 *Apo-Ident* customers from 15 batches from the substance/substance group *Sorbitan trioleate*.

Supplier	Substance	Batch	Spectra
Caelo	Sorbitan trioleate	12171408	2
Caelo	Sorbitan trioleate	11284607	1
Gehe	Sorbitan trioleate	12171408	1

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sorbitan trioleate	13317212	5
Caelo	Sorbitan trioleate	15064903	1
Caelo	Sorbitan trioleate	15064901	1
Caelo	Sorbitan trioleate	14218205	1
Caesar&Loretz GmbH	Sorbitan trioleate	15064903	1
Caelo	Sorbitan trioleate	15182502	1
Caesar & Lorenz GmbH	Sorbitan trioleate	15337404	1
Caelo	Sorbitan trioleate	11284608	1
Caelo	Sorbitan trioleate	11284603	1
Caesar & Loretz GmbH	Sorbitan trioleate	12171405	1
Caelo	Sorbitan trioleate	12171405	1
Caelo	Sorbitan trioleate	13317204	2
Caelo	Sorbitan trioleate	1217408	1
Caelo	Sorbitan trioleate	13317209	1
Caelo	Sorbitan trioleate	11284601	1

- 58 417 spectra from 332 *Apo-Ident* customers from a total of 20 077 batches from a further 328 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 *Sorbitan trioleate* 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 *Sorbitan trioleate* 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	119	0	34 225
Type B	0	37	0	63 557
Type C	0	24	0	58 417

The substance/substance group *Sorbitan trioleate* 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 % (> 99.9691 %)	100.0000 % (> 94.9580 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 83.7838 %)
Type C	100.0000 % (> 99.5967 %)	100.0000 % (> 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.

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
31031	31031	0.00	26.18
31130	31031	7.77	30.27
31459	31031	5.51	29.01

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Spearmint oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30668-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Spearmint oil; Menthae crispae aetheroleum; Oleum menthae crispae

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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
Caelo	Spearmint oil	11346805	30668	40	20111206
Caelo	Spearmint oil	13363904	31303	40	1407357
Caelo	Spearmint oil	13363904	31419	40	20131118

Validation samples

A total of 156 379 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 *Spearmint oil*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Spearmint oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Spearmint oil	13363904	31419 [†]	20
Caelo	Spearmint oil	161284	32205	40

- 63 534 spectra from a total of 1475 batches from further 439 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 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Spearmint oil*.

Supplier	Substance	Batch	Spectra
Noweda	Spearmint oil	11346805	1
Caelo	Spearmint oil	14147608	1
Caelo	Spearmint oil	12206910	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
Caelo	Spearmint oil	12206913	1
Caelo	Spearmint oil	13093402	1
Sanacorp	Spearmint oil	13093402	1

- 58 435 spectra from 332 *Apo-Ident* customers from a total of 20 087 batches from a further 328 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	120	0	34 224
Type B	0	60	0	63 534
Type C	0	6	0	58 435

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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.5978 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30668	31303	11.98	39.71
31303	31303	0.00	40.76
31419	31303	7.15	42.88

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Spirit of ether**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30707-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Spirit of ether; Spiritus aethereus

Special notes

When selecting the *Spirit of ether* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Spirit of ether*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Spirit of ether	12074603	30707	40	20120320
Caelo	Spirit of ether	13131805	31207	40	1403111

Validation samples

A total of 156 379 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 *Spirit of ether*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 1 reference samples from the substance/substance group *Spirit of ether*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Spirit of ether	15442201	32566	40

- 63 554 spectra from a total of 1476 batches from further 439 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 3 *Apo-Ident* customers from 6 batches from the substance/substance group *Spirit of ether*.

Supplier	Substance	Batch	Spectra
Caelo	Spirit of ether	13131805	2
Caelo	Spirit of ether	12074603	2
Caelo	Spirit of ether	14339702	2
Caelo	Spirit of ether	13131807	1
Caelo	Spirit of ether	11375509	1
Caelo	Spirit of ether	11375512	1

- 58 432 spectra from 332 *Apo-Ident* customers from a total of 20 086 batches from a further 328 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 *Spirit of ether* 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 *Spirit of ether* 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	34 264
Type B	0	40	0	63 554
Type C	0	8	1	58 432

The substance/substance group *Spirit of ether* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.5973 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30707	31207	6.31	122.07
31207	31207	0.00	129.62

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Spirit soap**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30546-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Spirit soap; Spiritus saponatus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Spirit soap*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Spirit soap	12247110	31153	40	1403401
Caelo	Spirit soap	13278409	31393	40	20130829

Validation samples

A total of 156 379 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 *Spirit soap*. These samples are listed above in the [calibration samples](#) section.
- 34 264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Spirit soap*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Spirit soap	11265306	30546	40
Caelo	Spirit soap	11265302	30588	40

- 63 514 spectra from a total of 1475 batches from further 439 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.

- 70 spectra from 27 *Apo-Ident* customers from 33 batches from the substance/substance group *Spirit soap*.

Supplier	Substance	Batch	Spectra
Caelo	Spirit soap	13278409	5
Caelo	Spirit soap	12247108	5
Caelo	Spirit soap	9031501	1
Caelo	Spirit soap	6081516	1
Caelo	Spirit soap	13278402	4
Caelo	Spirit soap	12247109	2

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Supplier	Substance	Batch	Spectra
Caelo	Spirit soap	12121402	1
Caelo	Spirit soap	12247110	6
Caelo	Spirit soap	13278403	6
Caelo	Spirit soap	13278405	3
Caelo	Spirit soap	13278408	2
Caelo	Spirit soap	14212706	5
Anzag	Spirit soap	13278409	1
Caelo	Spirit soap	14212703	1
Caelo	Spirit soap	14212710	1
Caelo	Spirit soap	14212714	1
Caelo	Spirit soap	14212716	1
Caelo	Spirit soap	14364901	1
Caelo	Spirit soap	14364902	3
Caesar&Lorenz	Spirit soap	14364906	1
Caelo	Spirit soap	14364904	3
Caelo	Spirit soap	14364906	2
Caelo	Spirit soap	16069902	1
Caelo	Spirit soap	16130202	2
Caelo	Spirit soap	14364907	1
Caelo	Spirit soap	3091306	1
Caelo	Spirit soap	9172002	1
Caelo	Spirit soap	10121303	1
Caelo	Spirit soap	12247102	1
Caelo	Spirit soap	12247104	1
Caelo	Spirit soap	12247107	1
Caelo	Spirit soap	12247105	1
Caelo	Spirit soap	27072013	1
Caelo	Spirit soap	2712Q-02323	1
Caelo	Spirit soap	3913U-02323	1

- 58 371 spectra from 332 *Apo-Ident* customers from a total of 20 060 batches from a further 328 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 *Spirit soap* 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 *Spirit soap* 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	34 264
Type B	0	79	1	63 514
Type C	0	61	9	58 371

The substance/substance group *Spirit soap* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9711 %)	98.7500 % (> 95.0000 %)
Type C	100.0000 % (> 99.5964 %)	87.1429 % (> 82.8571 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31153	31153	0.00	43.20
31393	31153	3.19	44.27

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Spruce needle oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31414-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Spruce needle oil; Oleum pini sibiricum; Piceae aetheroleum

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Spruce needle oil	13152004	31414	40	1412281
Caelo	Spruce needle oil	13152004	31618	40	20130617
Caelo	Spruce needle oil	14348607	31787	40	20141202

Validation samples

A total of 156 379 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 *Spruce needle oil*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 3 reference samples from the substance/substance group *Spruce needle oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Spruce needle oil	13152004	31618 [†]	20
Caelo	Spruce needle oil	14348607	31787 [†]	20
Caelo	Spruce needle oil	163511	33095	40

- 63 514 spectra from a total of 1474 batches from further 439 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 *Spruce needle oil*.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Spruce needle oil	14348607	1
Caelo	Spruce needle oil	13389508	1
Taoasis	Spruce needle oil	22336-122331	1

- 58 438 spectra from 332 *Apo-Ident* customers from a total of 20 089 batches from a further 328 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* 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* 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	34 224
Type B	0	80	0	63 514
Type C	0	2	1	58 438

The substance/substance group *Spruce needle 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5993 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31414	31414	0.00	33.39
31618	31414	2.25	33.19
31787	31414	5.25	32.57

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Squalane**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 31327-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Squalane; Squalanum

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Squalane*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Squalane	13202603	31327	40	1504359
Caelo	Squalane	13202603	31329	40	20130809
Caelo	Squalane	14330704	32075	40	9465
Caelo	Squalane	16030504	32302	40	20160205

Validation samples

A total of 156379 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 *Squalane*. These samples are listed above in the [calibration samples](#) section.
- 34184 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 1 reference samples from the substance/substance group *Squalane*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Squalane	13202603	31328	40

- 63554 spectra from a total of 1476 batches from further 439 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 2 batches from the substance/substance group *Squalane*.

Supplier	Substance	Batch	Spectra
Kaden	Squalane		2
Testsubstanz Saficalcan	Squalane	3104	1

- 58 438 spectra from 332 *Apo-Ident* customers from a total of 20 091 batches from a further 328 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 *Squalane* 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 *Squalane* 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	34 184
Type B	0	40	0	63 554
Type C	0	0	3	58 438

The substance/substance group *Squalane* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.5993 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31327	31327	0.00	12.55
31329	31327	1.88	12.29
32075	32075	0.00	14.51
32302	32075	2.85	12.55

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Strawberry aroma**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30643-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Strawberry aroma

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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	20130801
Caelo	Strawberry aroma	15411807	32814	40	20151130
Caelo	Strawberry aroma	15411807	32838	40	1704074

Validation samples

A total of 156 379 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 *Strawberry aroma*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 3 reference samples from the substance/substance group *Strawberry aroma*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Strawberry aroma	14311215	32567	40
Caelo	Strawberry aroma	14311215	32837	40
Caelo	Strawberry aroma	170246	33056	40

- 63 474 spectra from a total of 1475 batches from further 439 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 10 *Apo-Ident* customers from 13 batches from the substance/substance group *Strawberry aroma*.

Supplier	Substance	Batch	Spectra
Caelo	Strawberry aroma	9101405	1
Caelo	Strawberry aroma	12183513	4
Caelo	Strawberry aroma	13252405	1
Caelo	Strawberry aroma	13252407	1
Caelo	Strawberry aroma	14311204	1

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Supplier	Substance	Batch	Spectra
Caelo	Strawberry aroma	13252417	1
Caelo	Strawberry aroma	14311209	3
Caelo	Strawberry aroma	15411805	1
Caelo	Strawberry aroma	11178813	1
Caelo	Strawberry aroma	14311215	1
Caelo	Strawberry aroma	12183504	2
Caelo	Strawberry aroma	10184917	1
Caelo	Strawberry aroma	12183511	1

- 58 422 spectra from 332 *Apo-Ident* customers from a total of 20 079 batches from a further 328 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this [chemometric model](#), the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in [Appendix C](#).

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	160	0	34 184
Type B	0	120	0	63 474
Type C	0	19	0	58 422

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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.5968 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30643	30643	0.00	19.13
31395	30643	4.70	23.02
32814	30643	2.03	21.13
32838	32838	0.00	20.49

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Syrups**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30753-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Syrups; Althae sirupus (konserviert); Cherry syrup (conserved); Ipecacuanha syrup (NRF 19.1); Marshmallow syrup (conserved); Raspberry syrup (conserved); Ribwort plantain syrup (conserved); Sirupus althaeae (konserviert); Sirupus cerasi (konserviert); Sirupus ipecacuanhae; Sirupus plantaginis lanceolatae; Sirupus rubi idaei; Sirupus simplex; Sorbitol solution 70% (non-crystallizing); Sorbitolum liquidum non cristallisabile; Sugar syrup DAB

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Syrups*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Marshmallow syru...	12067103	30753	40	20120312
Caelo	Sorbitol solutio...	12124910	30870	40	20120525

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ribwort plantain...	11380011	30897	60	20120112
Caelo	Raspberry syrup ...	13122003	31051	40	1402567
Caelo	Sorbitol solutio...	13060206	31124	40	20130306
Caelo	Marshmallow syru...	12303106	31147	40	1404662
Caelo	Cherry syrup (co...	13278301	31155	40	1402568
apomix	Sugar syrup DAB	73A101013	31175	40	1403164
Fagron	Ipecacuanha syru...	13G23-M02	31181	40	1404013
Caelo	Ribwort plantain...	13152307	31218	40	1404663
Caelo	Sorbitol solutio...	14034706	31353	40	8780
Caelo	Sugar syrup DAB	14134301	31355	40	20140514
Caelo	Cherry syrup (co...	14034503	31359	40	20140131
Caelo	Marshmallow syru...	13410907	31365	40	20140318
Caelo	Raspberry syrup ...	14114303	31467	40	20140411
Euro OTC	Raspberry syrup ...	1508015	31773	40	20150814*
Euro OTC	Raspberry syrup ...	1511024	31802	40	20150511*
Caelo	Sugar syrup DAB	153348	31877	40	20151014*
Euro OTC	Raspberry syrup ...	1605008	32284	40	20160513*
Euro OTC	Raspberry syrup ...	1701022	32984	40	20170126*
Caelo	Cherry syrup (co...	163453	33099	40	20161221*
Fagron	Ipecacuanha syru...	02B200616	33263	40	20160627

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 900 spectra of 22 reference samples from the substance/substance group *Syrups*. These samples are listed above in the [calibration samples](#) section.
- 33 444 spectra from a total of 776 batches from further 218 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 810 spectra of 24 reference samples from the substance/substance group *Syrups*.

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

Supplier	Substance	Batch	Sample ID	Spectra
zu erfassen	Raspberry syrup (conserved)	pending	30176	30
Caelo	Cherry syrup (conserved)	10194902	30235	40
apomix	Sugar syrup DAB	52A150711	30401	40
apomix	Sugar syrup DAB	12A010212	30443	40
Caelo	Cherry syrup (conserved)	11168902	30478	40
Fagron	Ipecacuanha syrup (NRF 19.1)	11J20-M02	30484	40
Caelo	Sorbitol solution 70% (non-c...)	14034706	31353 [†]	20
Caelo	Sugar syrup DAB	14134301	31355 [†]	20
Caelo	Cherry syrup (conserved)	14034503	31359 [†]	20
Caelo	Raspberry syrup (conserved)	14114303	31467 [†]	20
Euro OTC	Raspberry syrup (conserved)	1508015	31773 [†]	20
Euro OTC	Raspberry syrup (conserved)	1511024	31802 [†]	20
Caelo	Sugar syrup DAB	153348	31877 [†]	20
Euro OTC	Raspberry syrup (conserved)	1603007	32193	40
Caelo	Marshmallow syrup (conserved)	161233	32210	40
Caelo	Raspberry syrup (conserved)	161516	32213	40
Caelo	Marshmallow syrup (conserved)	160775	32215	40
Caelo	Sorbitol solution 70% (non-c...)	160788	32217	40
Euro OTC	Sorbitol solution 70% (non-c...)	1604020	32277	40
Caelo	Marshmallow syrup (conserved)	162136	32335	40
Euro OTC	Raspberry syrup (conserved)	1608003	32705	40
Euro OTC	Raspberry syrup (conserved)	1610026	32833	40
Caelo	Raspberry syrup (conserved)	163454	33092	40
Euro OTC	Sorbitol solution 70% (non-c...)	1702011	33228	40

- 62 784 spectra from a total of 1454 batches from further 434 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.

- 641 spectra from 126 *Apo-Ident* customers from 356 batches from the substance/substance group *Syrups*.

Supplier	Substance	Batch	Spectra
Caelo	Marshmallow syrup (conserved)	1548604	1
Caelo	Marshmallow syrup (conserved)	13212910	1
Caelo	Marshmallow syrup (conserved)	14102602	1
Caelo	Marshmallow syrup (conserved)	14364804	1
Caelo	Marshmallow syrup (conserved)	12303101	1
Caelo	Marshmallow syrup (conserved)	15418604	1
Caelo	Marshmallow syrup (conserved)	13410909	1
Caelo	Marshmallow syrup (conserved)	13212909	2
Caelo	Marshmallow syrup (conserved)	12303106	2
Sanacorp	Marshmallow syrup (conserved)	13212909	1
Caelo	Marshmallow syrup (conserved)	13410907	1
Caelo	Raspberry syrup (conserved)	3121404	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
Caelo	Raspberry syrup (conserved)	4101405	1
Caelo	Raspberry syrup (conserved)	5021510	1
Euro OTC	Raspberry syrup (conserved)	11081402	1
Caelo	Raspberry syrup (conserved)	13051501	1
Euro OTC	Raspberry syrup (conserved)	1310016-01	9
Euro OTC	Raspberry syrup (conserved)	1306006-01	3
Caelo	Raspberry syrup (conserved)	13338001	6
Caelo	Raspberry syrup (conserved)	13393601	3
Caelo	Raspberry syrup (conserved)	13393602	3
Euro OTC	Raspberry syrup (conserved)	1406031-01	3
Euro OTC	Raspberry syrup (conserved)	140300201	1
noweda	Raspberry syrup (conserved)	13393605	1
Caelo	Raspberry syrup (conserved)	140903901	1
Caelo	Raspberry syrup (conserved)	14114303	1
Eurho/Phönix	Raspberry syrup (conserved)	1409039-01	1
Caelo	Raspberry syrup (conserved)	14114304	4
Caelo	Raspberry syrup (conserved)	14114305	3
Phönix	Raspberry syrup (conserved)	14114303	2
phoenix 14.11.14	Raspberry syrup (conserved)	14114306	1
Caelo	Raspberry syrup (conserved)	14114306	2
Caelo	Raspberry syrup (conserved)	14243401	1
Caelo	Raspberry syrup (conserved)	14243403	1
Caelo	Raspberry syrup (conserved)	14243405	3
Eurho/Phönix	Raspberry syrup (conserved)	1504011-01	2
Caelo	Raspberry syrup (conserved)	14371106	1
Noweda 04.08.15	Raspberry syrup (conserved)	1501011-01	1
Caelo	Raspberry syrup (conserved)	14371108	1
Euro OTC	Raspberry syrup (conserved)	1508015-01	2
Fagron	Raspberry syrup (conserved)	1501011-01	1
Euro OTC	Raspberry syrup (conserved)	1504011-01	1
Euro OTC	Raspberry syrup (conserved)	1511023-01	3
Euro OTC	Raspberry syrup (conserved)	1511024-01	2
Caelo	Raspberry syrup (conserved)	15149202	3
Caelo	Raspberry syrup (conserved)	15149202	1
Caelo	Raspberry syrup (conserved)	15149201	1
Caesar & Loretz	Raspberry syrup (conserved)	15149203	1
Caelo	Raspberry syrup (conserved)	15149205	5
Caelo	Raspberry syrup (conserved)	15320801	1
Caesar&Loretz	Raspberry syrup (conserved)	15320801	1
Caelo	Raspberry syrup (conserved)	15320804	1
Caelo	Raspberry syrup (conserved)	15320803	1
Euro OTC	Raspberry syrup (conserved)	1603007-01	3
Caesar&Loretz	Raspberry syrup (conserved)	15320804	1
Caelo	Raspberry syrup (conserved)	16003601	2
Caelo	Raspberry syrup (conserved)	15320813	1
Euro OTC	Raspberry syrup (conserved)	1605008-01	2
Caesar&Loretz	Raspberry syrup (conserved)	16003602	1
Caelo	Raspberry syrup (conserved)	11021405	1
Caesar & Loretz	Raspberry syrup (conserved)	16151602	1
noweda	Raspberry syrup (conserved)		1
Caelo	Raspberry syrup (conserved)	13194301	4
Caelo	Raspberry syrup (conserved)	1081201	1
Caelo	Raspberry syrup (conserved)	8021301	1
Caelo	Raspberry syrup (conserved)	4071203	1
Caelo	Raspberry syrup (conserved)	3011301	1
Eurho / Sanacorp	Raspberry syrup (conserved)	1110025-01	2
Caelo	Raspberry syrup (conserved)	1105022-01	1
Caelo	Raspberry syrup (conserved)	11291404	1
Caelo	Raspberry syrup (conserved)	11016508	1
Caelo	Raspberry syrup (conserved)	12038502	2

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Supplier	Substance	Batch	Spectra
phönix	Raspberry syrup (conserved)	12038501	1
Caelo	Raspberry syrup (conserved)	11363004	1
Caelo	Raspberry syrup (conserved)	12038501	3
Caelo	Raspberry syrup (conserved)	11169003	1
Caelo	Raspberry syrup (conserved)	12038505	1
Euro OTC	Raspberry syrup (conserved)	1205001-01	4
EuRho	Raspberry syrup (conserved)	1205001-01	3
Anzag 31.10.12	Raspberry syrup (conserved)	1205001-01	1
Euro OTC	Raspberry syrup (conserved)	1210004-01	14
Noweda	Raspberry syrup (conserved)	1210004-01	1
EuRho Anzag	Raspberry syrup (conserved)	1210004-01	1
Caelo	Raspberry syrup (conserved)	12161703	1
Caelo	Raspberry syrup (conserved)	12161705	4
Caelo	Raspberry syrup (conserved)	12121203	1
Caelo	Raspberry syrup (conserved)	1210004-01	1
Anzag 13.11.12	Raspberry syrup (conserved)	12283101	1
Caelo	Raspberry syrup (conserved)	12283101	3
Caelo	Raspberry syrup (conserved)	12283102	1
Caelo	Raspberry syrup (conserved)	12283103	4
Sanacorp	Raspberry syrup (conserved)	12283103	3
Caelo	Raspberry syrup (conserved)	12367601	1
Caelo	Raspberry syrup (conserved)	12367602	8
Gehe	Raspberry syrup (conserved)	12367602	1
Euro OTC	Raspberry syrup (conserved)	1302023-01	2
EuRho/Sanacorp	Raspberry syrup (conserved)	1302026-01	1
jenne eurho	Raspberry syrup (conserved)	1302026-01	1
Caelo	Raspberry syrup (conserved)	1302026-01	3
Euro OTC	Raspberry syrup (conserved)	1302026-01	3
Caelo	Raspberry syrup (conserved)	13122001	7
Caelo	Raspberry syrup (conserved)	13122002	1
Euro OTC	Raspberry syrup (conserved)	13802025-01	1
Caesar & Loretz/ Noweda	Raspberry syrup (conserved)	13122003	1
Caelo	Raspberry syrup (conserved)	13194302	1
Caelo	Raspberry syrup (conserved)	13122003	1
Phoenix	Raspberry syrup (conserved)	13338001	1
Phönix	Raspberry syrup (conserved)	141114303	1
Caelo	Raspberry syrup (conserved)	15051312	1
Caelo	Raspberry syrup (conserved)	18111308	1
Caelo	Raspberry syrup (conserved)	24081201	1
Caelo	Raspberry syrup (conserved)	2x13122001	1
Caelo	Raspberry syrup (conserved)	15071302	1
Caelo	Raspberry syrup (conserved)	17101202	1
Caelo	Raspberry syrup (conserved)	24091302	1
Caelo	Ipecacuanha syrup (NRF 19.1)	13G23-M02	1
Fagron	Ipecacuanha syrup (NRF 19.1)	14D17-M01	1
Fagron	Ipecacuanha syrup (NRF 19.1)	13G23-M02	1
Fagron	Ipecacuanha syrup (NRF 19.1)	15C11-M08	2
Fagron	Ipecacuanha syrup (NRF 19.1)	11B10-M01	1
Phönix	Cherry syrup (conserved)	14114304	1
Caelo	Cherry syrup (conserved)	109212258	1
Caelo	Cherry syrup (conserved)	12367501	1
Caelo	Cherry syrup (conserved)	14034502	1
Caelo	Cherry syrup (conserved)	11168902	1
Caelo	Cherry syrup (conserved)	14034503	1
Caelo	Cherry syrup (conserved)	13278301	1
Caelo	Cherry syrup (conserved)	13166201	1
Anzag	Cherry syrup (conserved)	11291603	1
Sanacorp	Raspberry syrup (conserved)	14243405	1
Caelo	Raspberry syrup (conserved)	14114302	1
Caelo	Raspberry syrup (conserved)	14371105	1

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Supplier	Substance	Batch	Spectra
Caelo	Raspberry syrup (conserved)	14371107	1
Gehe	Raspberry syrup (conserved)	12161702	1
Euro OTC	Raspberry syrup (conserved)	121000401	1
A.H.D.	Raspberry syrup (conserved)	12367602	2
Euro OTC	Raspberry syrup (conserved)	1302026-01-335031904	1
AHD	Raspberry syrup (conserved)	13122001	1
Sanacorp	Raspberry syrup (conserved)	13194301	1
apomix/Phönix	Sugar syrup DAB	2A130116	1
apomix/Phönix	Sugar syrup DAB	9A280116	1
Apomix/Anzag	Sugar syrup DAB	1314I-02263	1
Apomix/Gehe	Sugar syrup DAB	15A100215	1
Caelo	Sugar syrup DAB	15427102	1
Apomix/Gehe	Sugar syrup DAB	9A030214	2
Caelo	Sugar syrup DAB	16214002	1
Caelo	Sugar syrup DAB	16091501	1
Gutenberg-Apotheke	Sugar syrup DAB	18A030314	1
Apomix	Sugar syrup DAB	21A050314	3
Caelo	Sugar syrup DAB	16214101	1
Apomix/Gehe	Sugar syrup DAB	32A240415	1
Apomix/Phönix	Sugar syrup DAB	49A020715	2
Apomix/Gehe	Sugar syrup DAB	60A020914	1
Apommix-Sanacorp	Sugar syrup DAB	51A090713-3399310141	1
Phoenix/Apomix	Sugar syrup DAB	29A220313	1
Apomix/Gehe	Sugar syrup DAB	81A251114	1
Apomix/Gehe	Sugar syrup DAB	o9A030214	1
apomix/Phoenix	Sugar syrup DAB	20A280213	1
Anzag	Sugar syrup DAB	44A260612	1
Apomix/Sanacorp	Sugar syrup DAB	66A110913-3442311102	1
apomix/Phoenix	Sugar syrup DAB	73A101013	3
Caelo	Sorbitol solution 70% (non-c...	3031404	1
Caelo	Sorbitol solution 70% (non-c...	12/18-N09	1
Euro OTC	Sorbitol solution 70% (non-c...	1309026-01	3
Euro OTC	Sorbitol solution 70% (non-c...	1207012-02	1
Caelo	Sorbitol solution 70% (non-c...	13060204	4
Ichthyol/Gehe	Sorbitol solution 70% (non-c...	1309026-01	1
Phoenix	Sorbitol solution 70% (non-c...	1309026-02	1
Caelo	Sorbitol solution 70% (non-c...	1309026-01	2
Euro OTC	Sorbitol solution 70% (non-c...	1309026-02	4
Caelo	Sorbitol solution 70% (non-c...	13233801	2
Caelo	Sorbitol solution 70% (non-c...	13233803	3
Caelo	Sorbitol solution 70% (non-c...	13233807	3
Caelo	Sorbitol solution 70% (non-c...	13233804	1
Caelo	Sorbitol solution 70% (non-c...	13233808	3
Caelo	Sorbitol solution 70% (non-c...	13233810	4
Gehe	Sorbitol solution 70% (non-c...	13233810	1
Fagron	Sorbitol solution 70% (non-c...	13E24-B01	2
Euro OTC	Sorbitol solution 70% (non-c...	1412031-01	3
Caelo	Sorbitol solution 70% (non-c...	14034702	1
Fagron	Sorbitol solution 70% (non-c...	13J04-B01-289676	1
Caelo	Sorbitol solution 70% (non-c...	14034706	1
Euro OTC	Sorbitol solution 70% (non-c...	1412031-02	1
Caelo	Sorbitol solution 70% (non-c...	14169403	3
Euro OTC	Sorbitol solution 70% (non-c...	141203101	1
Caelo	Sorbitol solution 70% (non-c...	14169409	2
Caelo	Sorbitol solution 70% (non-c...	14298101	5
Caelo	Sorbitol solution 70% (non-c...	14298102	3
Caelo	Sorbitol solution 70% (non-c...	15159302	5
Caelo	Sorbitol solution 70% (non-c...	15159301	1
Caelo	Sorbitol solution 70% (non-c...	15175306	1
Caelo	Sorbitol solution 70% (non-c...	15175310	3

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Supplier	Substance	Batch	Spectra
Caelo	Sorbitol solution 70% (non-c...	15175307	1
Caelo	Sorbitol solution 70% (non-c...	1519302	1
Caelo	Sorbitol solution 70% (non-c...	15437907	1
Euro OTC	Sorbitol solution 70% (non-c...	1604020-01	2
Fagron	Sorbitol solution 70% (non-c...	29081505	1
Fagron	Sorbitol solution 70% (non-c...	21081406	1
Caelo	Sorbitol solution 70% (non-c...	16078807	1
Fagron	Sorbitol solution 70% (non-c...	2013M-02299	1
Caelo	Sorbitol solution 70% (non-c...	2071306	1
Caelo	Sorbitol solution 70% (non-c...	8051306	1
Caelo	Sorbitol solution 70% (non-c...	2071305	1
Gehe	Sorbitol solution 70% (non-c...	10323008	1
Caelo	Sorbitol solution 70% (non-c...	1102001-02	1
Euro OTC	Sorbitol solution 70% (non-c...	1102001-02	1
Caelo	Sorbitol solution 70% (non-c...	11255613	1
Fagron	Sorbitol solution 70% (non-c...	11G18-N14	1
Euro OTC	Sorbitol solution 70% (non-c...	1207012-01	4
Anzag	Sorbitol solution 70% (non-c...	120701201	1
Euro OTC	Sorbitol solution 70% (non-c...	120701201	1
Gehe	Sorbitol solution 70% (non-c...	1207012-01	1
Caelo	Sorbitol solution 70% (non-c...	1207012-01	2
Gehe	Sorbitol solution 70% (non-c...	1207012-02	1
EuRho	Sorbitol solution 70% (non-c...	1207012-02	1
Gehe	Sorbitol solution 70% (non-c...	120701202	1
Caelo	Sorbitol solution 70% (non-c...	12124903	2
Caelo	Sorbitol solution 70% (non-c...	12124905	1
Caelo	Sorbitol solution 70% (non-c...	12124906	2
Caelo	Sorbitol solution 70% (non-c...	12124908	2
Gehe	Sorbitol solution 70% (non-c...	12124910	1
Caelo	Sorbitol solution 70% (non-c...	12124912	4
Caelo	Sorbitol solution 70% (non-c...	12124914	5
Caelo	Sorbitol solution 70% (non-c...	12124915	1
Fagron	Sorbitol solution 70% (non-c...	12E08-N09	1
Gehe	Sorbitol solution 70% (non-c...	12E08-N09	1
Gehe	Sorbitol solution 70% (non-c...	12K07-N04	1
Caelo	Sorbitol solution 70% (non-c...	13060203	6
Gehe	Sorbitol solution 70% (non-c...	12118-N09	1
Caelo	Sorbitol solution 70% (non-c...	13060206	2
Caelo	Sorbitol solution 70% (non-c...	13060211	1
Fagron	Sorbitol solution 70% (non-c...	139026	1
Caelo	Sorbitol solution 70% (non-c...	22011306	1
Caelo	Sorbitol solution 70% (non-c...	28081301	1
Caelo	Sorbitol solution 70% (non-c...	26071209	1
EuRho/Phönix	Sorbitol solution 70% (non-c...	1412031-02	1
Caelo	Ribwort plantain syrup (cons...	13152308	3
Caelo	Ribwort plantain syrup (cons...	13152304	1
Caelo	Ribwort plantain syrup (cons...	14125702	1
Caelo	Ribwort plantain syrup (cons...	12347501	1
Sanacorp	Ribwort plantain syrup (cons...	13152303	1
Caelo	Ribwort plantain syrup (cons...	12347506	2
Caelo	Ribwort plantain syrup (cons...	13152305	1
Caelo	Ribwort plantain syrup (cons...	13152302	1
Apomix/Alliance Healthc...	Sugar syrup DAB	1A130116	1
Phönix Gotha	Sugar syrup DAB	1A130114	1
apomix	Sugar syrup DAB	2A130116	1
apomix/alliance healthc...	Sugar syrup DAB	3a150116	1
Apomix/Kehr	Sugar syrup DAB	3A150116	1
Apomix / Kehr	Sugar syrup DAB	5A220115	1
AMH Niemann/Phoenix	Sugar syrup DAB	3A270114	1
Apomix/ Noweda	Sugar syrup DAB	5A220115	1

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Supplier	Substance	Batch	Spectra
apomix/alliance healthc...	Sugar syrup DAB	3A150116	1
Apomix/Alliance Healthc...	Sugar syrup DAB	7A230115	1
Apomix PKH/V.d.L.	Sugar syrup DAB	7A310114	1
Apomix/Anzag	Sugar syrup DAB	1116E-02263	1
PKH-Halle/Sanacorp	Sugar syrup DAB	10A030214	1
APOMIX/ Alliance Health...	Sugar syrup DAB	7A310114	1
Apomix / Kehr	Sugar syrup DAB	11A120216	2
Alliance health	Sugar syrup DAB	11A280115	1
apomix/Kehr	Sugar syrup DAB	11A280115	2
AMH Niemann/Phoenix	Sugar syrup DAB	12A050214	1
Euro OTC	Sugar syrup DAB	13A150216	1
apomix	Sugar syrup DAB	13101405	1
Caelo	Sugar syrup DAB	14189102	1
Caelo	Sugar syrup DAB	14189101	1
Caelo	Sugar syrup DAB	14299801	4
Caelo	Sugar syrup DAB	14246001	1
Caelo	Sugar syrup DAB	14337004	1
Caelo	Sugar syrup DAB	15117002	1
Caelo	Sugar syrup DAB	15150602	1
Apomix/Anzag	Sugar syrup DAB	1515Q-02263	1
Apomix/Alliance Healthc...	Sugar syrup DAB	14A150216	1
JENNE	Sugar syrup DAB	16214101	1
Apomix/GEHE	Sugar syrup DAB	17A030314	1
apomix	Sugar syrup DAB	18081517	1
Apomix / Kehr	Sugar syrup DAB	18A030314	1
Apomix/Gehe	Sugar syrup DAB	18A030314	1
PKH Halle	Sugar syrup DAB	19A040314	1
apomix	Sugar syrup DAB	19A040314	1
Phoenix/apomix	Sugar syrup DAB	19A040314	1
Caelo	Sugar syrup DAB	20A270215	2
Caelo	Sugar syrup DAB	21A050314	1
Apomix/Anzag	Sugar syrup DAB	2112I-02263	1
apomix	Sugar syrup DAB	21A130315	1
Apomix	Sugar syrup DAB	22A050314	1
Caelo	Sugar syrup DAB	21A170316	1
Caelo	Sugar syrup DAB	22A130315	2
AMH Niemann GmbH & Co.KG	Sugar syrup DAB	22A130315	1
Apomix/Alliance Healthc...	Sugar syrup DAB	22A170316	1
Apomix/Alliance Healthc...	Sugar syrup DAB	25A170314	1
Caelo	Sugar syrup DAB	23A180316	1
Apomix / Kehr	Sugar syrup DAB	27A110416	3
rPhR Neidhar	Sugar syrup DAB	30A190416	1
Caelo	Sugar syrup DAB	30A190416	1
Apomix/Kehr	Sugar syrup DAB	30A200415	3
Apomix/Sanacorp	Sugar syrup DAB	35A070414	1
Apomix/Anzag	Sugar syrup DAB	37A03616	1
Alliance H.	Sugar syrup DAB	37/A030616	1
apomix	Sugar syrup DAB	37A220515	1
apomix/Noweda	Sugar syrup DAB	39A050614	2
Caelo	Sugar syrup DAB	38A190514	1
Phönix Neidhardt	Sugar syrup DAB	40A050614	1
apomix	Sugar syrup DAB	41A040716	1
apomix	Sugar syrup DAB	41A120615	1
apomix/Kehr	Sugar syrup DAB	43A110716	2
Apomix/Kehr	Sugar syrup DAB	42A120615	1
Apomix/Alliance Healthc...	Sugar syrup DAB	44A110716	1
Apomix / Kehr	Sugar syrup DAB	48A210714	1
Noweda / Apomix	Sugar syrup DAB	47A120613	1
apomix	Sugar syrup DAB	49A220714	1
apomix/Phoenix	Sugar syrup DAB	49A220714	2

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Supplier	Substance	Batch	Spectra
Apomix / Kehr	Sugar syrup DAB	49A290716	3
Apomix/Kehr	Sugar syrup DAB	51A010816	1
Apomix / Kehr	Sugar syrup DAB	50A020715	1
Apomix/Phönix	Sugar syrup DAB	51A070814	2
apomix	Sugar syrup DAB	55A130814	1
Apomix/Noweda	Sugar syrup DAB	57A180816	1
Apomix/Kehr	Sugar syrup DAB	57A260815	2
apomix	Sugar syrup DAB	57A140814	1
Apomix/Alliance Healthc. ...	Sugar syrup DAB	58A260815	1
apomix	Sugar syrup DAB	59A010914	1
Phoenix	Sugar syrup DAB	59A01914	1
apomix	Sugar syrup DAB	59A070814	1
Apomix / Kehr	Sugar syrup DAB	63A260916	2
Kehr/Apomix	Sugar syrup DAB	66A160914	2
Apomix/Alliance Healthc. ...	Sugar syrup DAB	68A131016	1
Apomix/Alliance Healthc. ...	Sugar syrup DAB	71A091015	1
Apomix/Alliance Healthc. ...	Sugar syrup DAB	68A230914	1
Apomix/Kehr	Sugar syrup DAB	72A091015	1
apomix/ Noweda	Sugar syrup DAB	72A091015	1
Apomix / Kehr	Sugar syrup DAB	74A241014	2
Caelo	Sugar syrup DAB	77A061114	1
Apomix/Anzag	Sugar syrup DAB	76A231015	2
apomix Fiebig	Sugar syrup DAB	77A261015	1
Phönix Gotha	Sugar syrup DAB	77A171013	1
Apomix/Kehr	Sugar syrup DAB	85A261115	1
Euro OTC	Sugar syrup DAB	80A061115	1
AMH Niemann GmbH	Sugar syrup DAB	85A261115	1
Apomix / Kehr	Sugar syrup DAB	86A051214	1
Caesar & Loretz GmbH	Sugar syrup DAB	86A051214	1
Noweda/Apomix	Sugar syrup DAB	87A051214	1
Apomix / Gehe	Sugar syrup DAB	87A071215	1
Kehr/Apomix	Sugar syrup DAB	88A121214	2
Apomix / Kehr	Sugar syrup DAB	88A12124	1
Apomix/Gehe	Sugar syrup DAB	89A111215	1
apomix/ Phönix	Sugar syrup DAB	93A231214	1
Phönix/apomix	Sugar syrup DAB	97A191213	2
Apomix / Noweda	Sugar syrup DAB	93A231214	1
apomix/Sanacorp	Sugar syrup DAB	96A161213	1
Apomix	Sugar syrup DAB	99A201213	1
AMH Niemann	Sugar syrup DAB	1A130114	1
Apomix	Sugar syrup DAB	1A140113	1
Apomix	Sugar syrup DAB	5A210113	1
Noweda	Sugar syrup DAB	11A060213	1
Apomix PKH/V.d.L.	Sugar syrup DAB	9A290113	1
apomix/ Phoenix	Sugar syrup DAB	11A060213	1
apomix	Sugar syrup DAB	11121305	1
Fagron	Sugar syrup DAB	13089R	1
Apomix	Sugar syrup DAB	12A010212	1
apomix/Phoenix	Sugar syrup DAB	15A210213	4
Caelo	Sugar syrup DAB	13A120213	1
Apomix	Sugar syrup DAB	17A270213	1
apomix	Sugar syrup DAB	16A210213	1
apomix/Phönix	Sugar syrup DAB	214050314	1
apomix	Sugar syrup DAB	20021307	1
apomix/ Phoenix	Sugar syrup DAB	21A010313	1
apomix/Phoenix	Sugar syrup DAB	21A010313	2
Caelo	Sugar syrup DAB	21A010313	1
apomix	Sugar syrup DAB	23081202	1
Apomix	Sugar syrup DAB	25A110313	1
Apomix	Sugar syrup DAB	25A200412	1

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Supplier	Substance	Batch	Spectra
Apomix/Phönix	Sugar syrup DAB	26A190313	1
Sanacorp/ PKH Halle	Sugar syrup DAB	29A110512	1
apomix	Sugar syrup DAB	27A270712	1
apomix	Sugar syrup DAB	27A200313	1
apomix/Phoenix	Sugar syrup DAB	29A220313	3
Apomix	Sugar syrup DAB	32A120413	1
Apomix/Phönix	Sugar syrup DAB	33A120413	3
Apomix/ Phönix	Sugar syrup DAB	34A240413	1
Apomix PKH/V.d.L.	Sugar syrup DAB	37A240413	2
apomix	Sugar syrup DAB	35A250512	1
PKH	Sugar syrup DAB	41A190612	1
Fagron	Sugar syrup DAB	38A250413	1
Apomix / Noweda	Sugar syrup DAB	41A230513	1
Nachprüfung	Sugar syrup DAB	42A220612	1
Phoenix	Sugar syrup DAB	43A040613	1
Apomix, Noweda	Sugar syrup DAB	43A040613	2
apomix	Sugar syrup DAB	46A030712	1
apomix	Sugar syrup DAB	43A260612	1
apomix	Sugar syrup DAB	45A050613	1
Caelo	Sugar syrup DAB	44A050613	1
Apomix	Sugar syrup DAB	47A050712	3
Apomix Anzag	Sugar syrup DAB	49A100712	1
Phönix Gotha	Sugar syrup DAB	51A090713	3
Apomix / Noweda	Sugar syrup DAB	51A090713	1
Gehe	Sugar syrup DAB	51A090713	1
Niemann GmbH & Co.KG	Sugar syrup DAB	53A080814	1
Phönix Gotha	Sugar syrup DAB		1
Apomix/ Gehe	Sugar syrup DAB	55A180712	2
Phönix/Apomix	Sugar syrup DAB	56A160813	3
Phönix/Apomix	Sugar syrup DAB	58A270712	1
noweda/Apomix	Sugar syrup DAB	56A160813	1
Caelo	Sugar syrup DAB	58A270712	1
Phönix Gotha	Sugar syrup DAB	59A220813	1
Gehe/ Apomix	Sugar syrup DAB	59A030812	1
apomix	Sugar syrup DAB	58A270712	1
apomix/Phoenix	Sugar syrup DAB	60A230813	2
Apomix PKH/V.d.L.	Sugar syrup DAB	64A050913	1
Phönix/ apomix	Sugar syrup DAB	66A110913	1
Phönix/apomix	Sugar syrup DAB	67A110913	2
Stred/apomix	Sugar syrup DAB	72A041013	2
apomix	Sugar syrup DAB	67A240912	1
Anzag 25.01.2013	Sugar syrup DAB	71A091012	1
AMH Niemann GmbH	Sugar syrup DAB	74A241014	1
Caelo	Sugar syrup DAB	76A171013	1
apomix/ Phoenix	Sugar syrup DAB	76A301012	1
Apomix/Noweda	Sugar syrup DAB	78A011112	1
Phönix/Apomix	Sugar syrup DAB	82A081112	3
Apomix	Sugar syrup DAB	81A-081112	1
apomix	Sugar syrup DAB	83A131112	1
Anzag 17.01.2013	Sugar syrup DAB	88A051212	1
apomix/Phoenix	Sugar syrup DAB	89A271113	1
Apomix/Gehe	Sugar syrup DAB	93A271212	1
apomix	Sugar syrup DAB	95A111213	1
Apomix	Sugar syrup DAB	94A281212	1

- 57 800 spectra from 332 *Apo-Ident* customers from a total of 19 744 batches from a further 322 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

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

Validation results

The validation runs checked whether the substance/substance group *Syrups* 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 *Syrups* 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	33 444
Type B	0	800	10	62 784
Type C	0	631	10	57 800

The substance/substance group *Syrups* 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 % (> 99.9689 %)	100.0000 % (> 99.3333 %)
Type B	100.0000 % (> 99.9710 %)	98.7654 % (> 98.3951 %)
Type C	100.0000 % (> 99.5963 %)	98.4399 % (> 97.9719 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30753	31147	3.49	48.07
30870	31353	8.04	23.45
30897	31877	3.50	44.45
31051	31051	0.00	32.32
31124	31353	2.04	24.68
31147	31147	0.00	48.95
31155	31155	0.00	31.60
31175	31175	0.00	46.46
31181	31181	0.00	43.46
31218	31218	0.00	40.22
31353	31353	0.00	24.97
31355	31175	1.98	46.90

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31359	31051	1.55	32.73
31365	31877	3.28	48.07
31467	31051	1.83	32.87
31773	31773	0.00	32.40
31802	31802	0.00	33.49
31877	31877	0.00	46.58
32284	32284	0.00	34.40
32984	32984	0.00	32.59
33099	33099	0.00	27.53
33263	31181	5.73	41.16

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Tea tree oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31023-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tea tree oil; Melaleuca alternifolia oleum; Oleum melaleuca alternifolia

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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
Caelo	Tea tree oil	12201303	31023	40	1404597
Caelo	Tea tree oil	13288914	31401	40	20130828
Caelo	Tea tree oil	14203203	31960	40	20140703

Validation samples

A total of 156 379 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 *Tea tree oil*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 59 spectra of 2 reference samples from the substance/substance group *Tea tree oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tea tree oil	244265	30306	39
Caelo	Tea tree oil	14203203	31960 [†]	20

- 63 535 spectra from a total of 1475 batches from further 439 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.

- 56 spectra from 24 *Apo-Ident* customers from 37 batches from the substance/substance group *Tea tree oil*.

Supplier	Substance	Batch	Spectra
Caelo	Tea tree oil	14203202	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
Caelo	Tea tree oil	11333516	1
primavera	Tea tree oil	5604136	1
Taoasis	Tea tree oil	41015006139	1
Caelo	Tea tree oil	11358910	1
Caelo	Tea tree oil	12201303	1
Caelo	Tea tree oil	12201304	3
Caelo	Tea tree oil	12201303	2
Caelo	Tea tree oil	12201311	3
Caelo	Tea tree oil	12201313	1
Apoth.Bauer&Co,Münch	Tea tree oil		2
Caelo	Tea tree oil	13099506	2
Caelo	Tea tree oil	13099510	1
Caelo	Tea tree oil	13288902	1
Caelo	Tea tree oil	14071604	1
Caelo	Tea tree oil	14203203	3
Caelo	Tea tree oil	14111201	1
Caelo	Tea tree oil	14302301	4
Caelo	Tea tree oil	14302302	1
Caelo	Tea tree oil	15051806	2
Ebert 01.09.2016	Tea tree oil	15337105	1
Minck	Tea tree oil	1511E-03093	1
Caelo	Tea tree oil	15337111	1
Taoasis	Tea tree oil	516495-108562	1
Taoasis	Tea tree oil	33152-112369	1
Taoasis	Tea tree oil	535627-110746	2
Taoasis	Tea tree oil	556031-114257	2
bauer und cie münchen	Tea tree oil		2
apotheker bauer& cie oHG	Tea tree oil	6548331306	1
Apotheker bauer	Tea tree oil		1
Bergland-Pharma/Anzag	Tea tree oil	C002685	1
Apoth.Bauer&Co,Münch	Tea tree oil	692624	1
Taoasis GmbH	Tea tree oil	98546	1
Sensient	Tea tree oil	C9663	1
Gehe	Tea tree oil	K203705	3
Bergland /Noweda	Tea tree oil	K302332	1
Bergland-Pharma/Anzag	Tea tree oil	C101782	1
Bergland / Noweda	Tea tree oil	P102633	1

- 58385 spectra from 332 *Apo-Ident* customers from a total of 20056 batches from a further 328 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	120	0	34224
Type B	0	50	9	63535
Type C	0	47	9	58385

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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	84.7458 % (> 79.6610 %)
Type C	100.0000 % (> 99.5964 %)	83.9286 % (> 78.5714 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31023	31023	0.00	50.89
31401	31023	25.99	48.92
31960	31023	7.64	52.26

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Texapon[®] CS paste**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30879-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Texapon[®] CS paste

Special notes

When selecting the *Texapon[®] CS paste* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Texapon[®] CS paste*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Texapon [®] CS paste	12292001	30879	40	20121010
Caelo	Texapon [®] CS paste	12292006	31113	40	20121010
Caelo	Texapon [®] CS paste	14087206	31562	40	1501415
Caelo	Texapon [®] CS paste	16268901	32821	40	20160915

Validation samples

A total of 156 379 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 *Texapon[®] CS paste*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 60 spectra of 2 reference samples from the substance/substance group *Texapon[®] CS paste*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Texapon [®] CS paste	14087206	31562 [†]	20
Caelo	Texapon [®] CS paste	16268901	32820	40

- 63 534 spectra from a total of 1475 batches from further 439 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 *Texapon[®] CS paste*.

Supplier	Substance	Batch	Spectra
Caelo	Texapon [®] CS paste	15177804	2
Caelo	Texapon [®] CS paste	1577804	1
Caelo	Texapon [®] CS paste	12292006	1
Caelo	Texapon [®] CS paste	12292007	1

[†]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*.

- 58 436 spectra from 332 *Apo-Ident* customers from a total of 20 088 batches from a further 328 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 *Texapon*[®] *CS 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 *Texapon*[®] *CS 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	34 184
Type B	0	60	0	63 534
Type C	0	5	0	58 436

The substance/substance group *Texapon*[®] *CS 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.5981 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30879	31562	10.62	28.47
31113	31562	7.82	23.28
31562	31562	0.00	24.44
32821	31562	6.32	17.66

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Thyme oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30206-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Thyme oil; Oleum thymi

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Thyme oil	12020518	31018	40	1407220
Caelo	Thyme oil	14225405	31566	40	20140822
Caelo	Thyme oil	15230104	32265	40	20150702
Caelo	Thyme oil	163279	33083	40	20161222*

Validation samples

A total of 156 379 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 *Thyme oil*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 120 spectra of 3 reference samples from the substance/substance group *Thyme oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Thyme oil	10078906	30206	40
Primavera	Thyme oil	9212141	31499	60
Caelo	Thyme oil	14225405	31566 [†]	20

- 63 474 spectra from a total of 1474 batches from further 439 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.

- 108 spectra from 54 *Apo-Ident* customers from 54 batches from the substance/substance group *Thyme 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.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Thyme oil	15402204	1
Caelo	Thyme oil	13044710	1
Caelo	Thyme oil	13044716	3
Caelo	Thyme oil	14225403	1
Bombastus	Thyme oil	283494	1
Caelo	Thyme oil	14225414	1
Caelo	Thyme oil	14225418	1
Caelo	Thyme oil	3313U-02023	1
Caelo	Thyme oil	12020515	1
Caelo	Thyme oil	12020514	5
Caelo	Thyme oil	13044705	1
Caelo	Thyme oil	12020518	7
Bombastus	Thyme oil	268010	2
Caelo	Thyme oil	13044707	4
Caelo	Thyme oil	6081401	1
Caelo	Thyme oil	10118603	1
Taoasis	Thyme oil	109378	1
PVL	Thyme oil	271112	1
Fagron	Thyme oil	10L20-N09	1
Caelo	Thyme oil	11275801	1
Caelo	Thyme oil	11275806	1
Caelo	Thyme oil	12020510	7
Fiebi 07.11.12 ek:8,48	Thyme oil	12020503	1
Phönix 03.12.12	Thyme oil	11275811	1
Caelo	Thyme oil	11275811	1
Anzag 27.12.12 ek:8,71	Thyme oil	12020510	2
Caelo	Thyme oil	12020503	4
Caelo	Thyme oil	12020511	1
Großhandel	Thyme oil	12165401	1
Caelo	Thyme oil	12165401	1
Caelo	Thyme oil	1221104	1
Caelo	Thyme oil	12201104	4
Caelo	Thyme oil	13021303	1
Caelo	Thyme oil	13044702	3
Caelo	Thyme oil	13044708	3
Bombastus	Thyme oil	13044708	1
Caelo	Thyme oil	13044709	1
GEHE 02.07.2014	Thyme oil	13044715	3
Caelo	Thyme oil	13044715	2
Caelo	Thyme oil	142225412	1
Caelo	Thyme oil	14071202	1
Caelo	Thyme oil	14225405	2
Caelo	Thyme oil	14225401	2
Caelo	Thyme oil	14225406	2
Caelo	Thyme oil	14225413	4
Caelo	Thyme oil	14225410	1
Caelo	Thyme oil	14225417	1
Caelo	Thyme oil	15230104	1
Caelo	Thyme oil	1540220	1
Caelo	Thyme oil	15402202	5
Caesar & Loretz/Noweda	Thyme oil	15402202	1
Caelo	Thyme oil	15402207	1
Caelo	Thyme oil	2615A-02023	1
Post-Apotheke	Thyme oil	268011	2
Taoasis	Thyme oil	28739-104426	1
Taoasis	Thyme oil	28739-106640	1
Taoasis	Thyme oil	31911-109378	1
Taoasis	Thyme oil	31911-110649	1
Euro OTC	Thyme oil		1
Fagron	Thyme oil	606549	1

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Supplier	Substance	Batch	Spectra
Caelo	Thyme oil	3211I-02023	1

- 58 333 spectra from 332 *Apo-Ident* customers from a total of 20 039 batches from a further 328 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* 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* 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	34 184
Type B	0	20	100	63 474
Type C	0	84	24	58 333

The substance/substance group *Thyme 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	16.6667 % (> 14.1667 %)
Type C	100.0000 % (> 99.5964 %)	77.7778 % (> 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.

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
31018	31018	0.00	45.54
31566	31018	7.28	46.99
32265	33083	12.08	39.04
33083	33083	0.00	44.15

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Triglycerides
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30647-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Triglycerides; Almond oil, refined; Amygdalae oleum raffinatum; Apricot kernel oil, refined; Arachidis oleum raffinatum; Avocado oil, refined; Avocado oleum raffinatum; Borage oil, refined, stabilised; Carthami oleum raffinatum; Codliver oil (type A); Corn oil, refined; Decyl oleate; Decylis oleas; Decylium oleinicum; Evening primrose oil, refined; Flaxseed oil, native; Grape seed oil, refined; Iecoris aselli oleum A; Jojoba oil, native; Laurel oil; Lecithinum e sojæ, liquidus; Lini oleum virginale; Macadamia oil, refined; Oenotherae oleum raffinatum; Oleum amygdalarum raffinatum; Oleum arachidis raffinatum; Oleum boraginis raffinatum; Oleum carthami; Oleum cucurbita semen; Oleum helianthi raffinatum; Oleum jecoris (Typ A); Oleum juglandis raffinatum; Oleum lauri expressum; Oleum lini; Oleum macadamiae raffinatum; Oleum maydis raffinatum; Oleum oenotherae raffinatum; Oleum olivarum nativum; Oleum omega-3 18/12; Oleum persea americana raffinatum; Oleum pruni armeniæ raffinatum; Oleum rapae raffinatum; Oleum sesami raffinatum; Oleum simmondsia chinensis; Oleum sojæ raffinatum; Oleum tritici raffinatum; Oleum vitis viniferae raffinatum; Oleyl oleate (stabilised); Oleylis oleas; Oleylium oleinicum; Olivæ oleum virginale; Olive oil, native; Omega-3-fish oil 18/12; Peanut oil, refined; Pumpkin seed oil, pressed; Rapae oleum raffinatum; Rapeseed oil, refined; Safflower oil, refined type I; Sesame oil, refined; Soy lecithin, liquid; Soy oil, refined; Sunflower oil, refined; Tritici aestivi oleum raffinatum; Walnut oil, refined; Wheatgerm oil, refined

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Triglycerides*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Rapeseed oil, re...	12054402	30647	40	20120321
Henry Lamotte	Omega-3-fish oil...	0123108	30679	40	20120613
Caelo	Oleyl oleate (st...	12220205	30754	40	20120803
Caelo	Apricot kernel o...	11346402	30840	40	20111214
Caelo	Evening primrose...	12325103	30855	40	20121107
Caelo	Oleyl oleate (st...	12220207	30863	40	20120803
Caelo	Sesame oil, refi...	12054508	30873	40	20120323
Caelo	Codliver oil (ty...	12062501	30878	40	20120411
Caelo	Safflower oil, r...	13011302	30981	80	1407318
Caelo	Corn oil, refined	12141511	31016	40	1407320
Euro OTC	Soy lecithin, li...	1305019-01	31034	40	20130603
Caelo	Grape seed oil, ...	13065302	31121	40	1407373
Caelo	Laurel oil	13024511	31122	40	1403397
Caelo	Macadamia oil, r...	13012102	31156	40	1407349
Caelo	Borage oil, refi...	13170606	31161	40	1407319
Bombastus	Flaxseed oil, na...	281489	31172	40	1407202
Henry Lamotte	Omega-3-fish oil...	0123780	31178	40	20130403
Caelo	Wheatgerm oil, r...	13011508	31210	40	1407215
Caelo	Rapeseed oil, re...	13011008	31215	40	1406536
Caelo	Walnut oil, refi...	13202401	31216	40	1406537
Caelo	Sunflower oil, r...	13011411	31217	40	1406538
Caelo	Peanut oil, refi...	13306106	31246	40	1406534
Caelo	Almond oil, refi...	13350007	31250	40	1407348
Caelo	Corn oil, refined	13249005	31274	40	1407347
Caelo	Jobba oil, native	13287709	31322	40	AR-14-FG-012487-01
Caelo	Flaxseed oil, na...	14087903	31326	40	20140401
Caelo	Pumpkin seed oil...	13358504	31332	40	AR-14-FG-012336-02
Caelo	Avocado oil, ref...	13361406	31336	40	AR-15-FG-002721-01
Caelo	Almond oil, refi...	14042704	31337	40	20140211
Caelo	Corn oil, refined	13249005	31344	40	20130819
Caelo	Peanut oil, refi...	14115404	31346	40	20140415
Caelo	Sesame oil, refi...	13397402	31350	40	AR-14-FG-012338-01
Caelo	Olive oil, native	14024409	31356	40	20140130
Caelo	Codliver oil (ty...	13396403	31361	40	AR-14-FG-012167-01
Caelo	Safflower oil, r...	13358705	31362	40	20131122
Caelo	Sunflower oil, r...	13225110	31374	40	20130813
Caelo	Apricot kernel o...	13357604	31375	40	1412121
Caelo	Rapeseed oil, re...	13236506	31376	40	20130806
Caelo	Soy oil, refined	13361305	31378	40	20131122
Caelo	Walnut oil, refi...	13364501	31380	40	20131122
Caelo	Decyl oleate	13378403	31382	40	AR-15-FG-000232-01
Caelo	Borage oil, refi...	14161904	31384	40	20140522
Caelo	Evening primrose...	14010915	31460	40	AR-14-FG-012898-01
Caelo	Jobba oil, native	13287709	31482	40	20130920
Caelo	Wheatgerm oil, r...	13261604	31491	40	1412119
Caelo	Oleyl oleate (st...	14005001	31496	40	AR-15-FG-001552-01
Caelo	Jobba oil, native	13287709	31519	40	20130920
Euro OTC	Soy lecithin, li...	1404022-01	31523	40	8779
Henry Lamotte	Omega-3-fish oil...	0124495	31540	40	20140325
Caelo	Evening primrose...	14258610	31572	40	AR-15-FG-002720-01
Euro OTC	Decyl oleate	1309018-01	31584	40	20131007
Euro OTC	Olive oil, native	1407052-02	31585	40	20140812
Euro OTC	Evening primrose...	1407002-02	31589	40	20140718
Caelo	Pumpkin seed oil...	14199402	31609	40	1507428

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macadamia oil, r...	14179304	31616	40	20140611
Caelo	Avocado oil, ref...	14363703	31662	40	20150114
Fagron	Codliver oil (ty...	14D16-B08-304341	31677	40	20140520
Euro OTC	Evening primrose...	1506001	31708	40	20150616*
Henry Lamotte	Omega-3-fish oil...	1000000642	31729	40	1601423
Caelo	Laurel oil	15216402	31745	40	20150717
Euro OTC	Almond oil, refi...	1510014	31770	40	20151022*
Euro OTC	Evening primrose...	1509005	31775	40	20150921*
Henry Lamotte	Omega-3-fish oil...	1000000642	31792	40	20150414
Euro OTC	Avocado oil, ref...	1501015	31801	40	20150121*
Fagron	Codliver oil (ty...	15A07-B05-304428	31825	40	20150116
Caelo	Laurel oil	15216401	31833	30	1606485
Caelo	Soy oil, refined	15239302	31834	40	20150817
Henry Lamotte	Omega-3-fish oil...	1000001175	31875	40	20150626
Caelo	Olive oil, native	161446	32195	40	20160524*
Caelo	Peanut oil, refi...	162495	32680	40	20160831*
Caelo	Apricot kernel o...	162361	32683	40	20160818*
Caelo	Wheatgerm oil, r...	16137403	32730	40	20160708
Caelo	Sunflower oil, r...	15422804	32745	40	20151218
Caelo	Grape seed oil, ...	16092402	32989	40	20160407
Caelo	Peanut oil, refi...	170428	33059	40	20170215*
Caelo	Apricot kernel o...	170555	33060	30	20170308*
Caelo	Flaxseed oil, na...	170467	33064	40	20170222*
Caelo	Avocado oil, ref...	170388	33067	40	20170209*
Caelo	Decyl oleate	170595	33070	40	20170308*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 3180 spectra of 79 reference samples from the substance/substance group *Triglycerides*. These samples are listed above in the [calibration samples](#) section.
- 31 164 spectra from a total of 723 batches from further 199 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

*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.

- 3342 spectra of 93 reference samples from the substance/substance group *Triglycerides*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Olive oil, native	90417099	30044	9
Caelo	Peanut oil, refined	90753159	30049	10
Caelo	Borage oil, refined, stabili...	9267308	30162	40
Caelo	Laurel oil	10185405	30168	40
Caelo	Grape seed oil, refined	10066303	30192	29
Caelo	Sunflower oil, refined	10159002	30200	37
Bombastus	Olive oil, native	254963	30226	20
Caelo	Peanut oil, refined	1081502	30227	10
Caelo	Olive oil, native	10314504	30249	40
Caelo	Almond oil, refined	11032604	30257	40
Caelo	Almond oil, refined	11032604	30259	40
Caelo	Avocado oil, refined	10215207	30270	40
Caelo	Corn oil, refined	10104608	30271	40
Caelo	Peanut oil, refined	11000503	30272	130
Caelo	Olive oil, native	10314508	30273	130
Caelo	Almond oil, refined	11032605	30274	130
Caelo	Avocado oil, refined	10215207	30275	130
Caelo	Olive oil, native	11063901	30288	50
Caelo	Avocado oil, refined	10215207	30290	32
Bombastus	Joboba oil, native	256221	30294	50
Taoasis	Macadamia oil, refined	4976601-92844	30308	40
Caelo	Joboba oil, native	252449	30314	40
Euro OTC	Soy lecithin, liquid	1006017-01	30321	30
Caelo	Peanut oil, refined	11163201	30331	40
Caelo	Avocado oil, refined	243981	30347	40
Henry Lamotte	Peanut oil, refined	5052601	30366	30
Statfold	Flaxseed oil, native	17732	30413	40
Caelo	Walnut oil, refined	10328802	30419	40
Bombastus	Flaxseed oil, native	269324	30522	40
Caelo	Wheatgerm oil, refined	11227305	30550	40
Caelo	Peanut oil, refined	14115404	31346 [†]	20
Caelo	Sesame oil, refined	13397402	31350 [†]	20
Caelo	Olive oil, native	14024409	31356 [†]	20
Caelo	Codliver oil (type A)	13396403	31361 [†]	20
Caelo	Safflower oil, refined type I	13358705	31362 [†]	20
Caelo	Evening primrose oil, refined	14010915	31460 [†]	20
Caelo	Joboba oil, native	13287709	31482 [†]	20
Caelo	Oleyl oleate (stabilised)	14005001	31496 [†]	20
Caelo	Joboba oil, native	13287709	31519 [†]	20
Euro OTC	Soy lecithin, liquid	1404022-01	31523 [†]	20
Henry Lamotte	Omega-3-fish oil 18/12	124495	31540 [†]	20
Caelo	Evening primrose oil, refined	14258610	31572 [†]	20
Euro OTC	Decyl oleate	1309018-01	31584 [†]	20
Euro OTC	Olive oil, native	1407052-02	31585 [†]	20
Euro OTC	Evening primrose oil, refined	1407002-02	31589 [†]	20
Caelo	Pumpkin seed oil, pressed	14199402	31609 [†]	20
Caelo	Macadamia oil, refined	14179304	31616 [†]	20
Henry Lamotte	Codliver oil (type A)	125348	31643	60
Caelo	Laurel oil	14176301	31657	15
Caelo	Avocado oil, refined	14363703	31662 [†]	20
Fagron	Codliver oil (type A)	14D16-B08-304341	31677 [†]	20
Euro OTC	Evening primrose oil, refined	1506001	31708 [†]	20
Henry Lamotte	Omega-3-fish oil 18/12	1000000642	31729 [†]	20
Caelo	Laurel oil	15216402	31745 [†]	20
Euro OTC	Almond oil, refined	1510014	31770 [†]	20
Euro OTC	Evening primrose oil, refined	1509005	31775 [†]	20

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Supplier	Substance	Batch	Sample ID	Spectra
Henry Lamotte	Omega-3-fish oil 18/12	1000000642	31792 [†]	20
Euro OTC	Avocado oil, refined	1501015	31801 [†]	20
Fagron	Codliver oil (type A)	15A07-B05-304428	31825 [†]	20
Caelo	Laurel oil	15216401	31833 [†]	30
Caelo	Soy oil, refined	15239302	31834 [†]	20
Henry Lamotte	Omega-3-fish oil 18/12	1000001175	31875 [†]	20
Euro OTC	Olive oil, native	1602022	32186	40
Euro OTC	Almond oil, refined	1603025	32188	40
Caelo	Decyl oleate	161071	32194	40
Caelo	Avocado oil, refined	161047	32197	40
Caelo	Almond oil, refined	161444	32198	40
Caelo	Walnut oil, refined	161007	32199	40
Caelo	Oleyl oleate (stabilised)	161049	32202	40
Caelo	Peanut oil, refined	161195	32206	40
Caelo	Avocado oil, refined	161859	32315	40
Caelo	Rapeseed oil, refined	161850	32316	40
Caelo	Safflower oil, refined type I	161849	32334	40
Euro OTC	Avocado oil, refined	1605034	32457	40
Euro OTC	Evening primrose oil, refined	1605027	32463	40
Caelo	Evening primrose oil, refined	162813	32682	40
Caelo	Borage oil, refined, stabili...	162660	32685	40
Caelo	Corn oil, refined	162603	32689	40
Caelo	Codliver oil (type A)	162739	32690	40
Caelo	Sunflower oil, refined	162758	32691	40
Euro OTC	Olive oil, native	1608006	32709	40
Caelo	Soy oil, refined	15239302	32729	40
Henry Lamotte	Omega-3-fish oil 18/12	1000002824	32734	40
Caelo	Grape seed oil, refined	16092401	32746	40
Caelo	Pumpkin seed oil, pressed	15410004	32783	40
Bombastus	Olive oil, native	306949	32990	40
Caelo	Olive oil, native	163274	33063	30
Caelo	Macadamia oil, refined	170556	33065	40
Caelo	Almond oil, refined	170422	33066	40
Caelo	Olive oil, native	170387	33068	40
Caelo	Corn oil, refined	170550	33069	40
Caelo	Sesame oil, refined	163125	33075	40
Caelo	Peanut oil, refined	163553	33085	40

- 60 252 spectra from a total of 1390 batches from further 415 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.

- 5388 spectra from 295 *Apo-Ident* customers from 1577 batches from the substance/substance group *Triglycerides*.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Almond oil, refined	13350001	13
Caelo	Almond oil, refined	13350003	14
Caelo	Almond oil, refined	14042703	6
Caelo	Almond oil, refined	14139305	2
Caelo	Almond oil, refined	14215807	1
Caelo	Almond oil, refined	14215806	7
Caelo	Almond oil, refined	14139310	12
Caelo	Almond oil, refined	14139311	6
Caelo	Almond oil, refined	14215816	1
Caelo	Almond oil, refined	15078404	8
Caelo	Almond oil, refined	15409712	5
Bombastus	Almond oil, refined	283800	2
Bombastus	Almond oil, refined	295615	1
Bombastus	Almond oil, refined	286253	1
Bombastus	Almond oil, refined	288471	3
Caelo	Almond oil, refined	12357112	3
Lamotte/Gehe	Almond oil, refined	5615001	1
Caelo	Almond oil, refined	13178004	14
Caelo	Almond oil, refined	13178002	13
Bombastus	Almond oil, refined	277971	5
Sanacorp	Almond oil, refined	12357103	1
Sanacorp	Almond oil, refined	13178004	1
Bombastus	Almond oil, refined	281040	4
Fagron	Almond oil, refined	5438301	2
Henry Lamotte/Gehe	Almond oil, refined	5415901	2
Caelo	Almond oil, refined	13236402	18
Henry Lamotte Oils	Almond oil, refined	5438302	5
Henry Lamotte/N/PZN:731...	Almond oil, refined	5438302	2
Caelo	Apricot kernel oil, refined	13253203	2
Primavera	Apricot kernel oil, refined	3612131	1
Bombastus	Apricot kernel oil, refined	274930	1
Caelo	Apricot kernel oil, refined	13011805	1
Caelo	Apricot kernel oil, refined	13011804	1
Caelo	Peanut oil, refined	13358803	13
Caelo	Peanut oil, refined	14115405	11
Caelo	Peanut oil, refined	14115406	15
Fagron	Peanut oil, refined	13G30-N05	8
Caelo	Peanut oil, refined	14246901	11
Caelo	Peanut oil, refined	12323205	3
Caelo	Peanut oil, refined	14355904	9
Euro OTC	Peanut oil, refined	5592601	1
Caelo	Peanut oil, refined	13306102	8
Caelo	Peanut oil, refined	12274305	3
Caelo	Peanut oil, refined	15015103	7
Sanacorp	Peanut oil, refined	13129203	1
Caelo	Peanut oil, refined	13306103	25
Bombastus	Peanut oil, refined	284286	4
Caelo	Avocado oil, refined	12248312	3
Caelo	Avocado oil, refined	13361407	2
Euro OTC	Avocado oil, refined	1304039-01	6
Euro OTC	Avocado oil, refined	1301017-01	1
Euro OTC	Avocado oil, refined	1405007-01	2
Caelo	Avocado oil, refined	13129108	5
Sanacorp	Avocado oil, refined	1304039-01	1
Euro OTC	Avocado oil, refined	1305046-01	4
Henry Lamotte Oils GmbH	Avocado oil, refined	1000001098	1
Caelo	Avocado oil, refined	15155206	2
Caelo	Avocado oil, refined	13129103	6
Lamotte GmbH	Avocado oil, refined	1000001451	1
Caelo	Avocado oil, refined	15268205	4

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Supplier	Substance	Batch	Spectra
Caelo	Avocado oil, refined	15426304	1
Caelo	Avocado oil, refined	15426305	2
Caelo	Avocado oil, refined	16104702	1
Caesar & Loretz/Noweda	Avocado oil, refined	15268203	1
Caelo	Avocado oil, refined	15268213	1
Bombastus	Avocado oil, refined	294183	2
Caelo	Avocado oil, refined	300403	1
Caelo	Avocado oil, refined	2515I-01960	1
Henry Lamotte Oils GmbH	Avocado oil, refined	125529	2
Caelo	Avocado oil, refined	15426306	1
Ebert u. Jacobi 16.0...	Avocado oil, refined	302706	1
Lamotte/Sanacorp	Avocado oil, refined	130214	1
Henry Lamotte Oils GmbH	Avocado oil, refined	130243	1
Euro OTC	Avocado oil, refined	2041404	1
Henry Lamotte/Sana	Avocado oil, refined	1000001098	1
Euro OTC	Avocado oil, refined	13111404	1
Phoenix 19.03.2014	Avocado oil, refined	13129102	1
Nachprüfung	Avocado oil, refined	13129103	2
Caelo	Avocado oil, refined	13129111	1
Phoenix 29.04.2014	Avocado oil, refined	13361406	1
Caelo	Avocado oil, refined	13361406	4
Großhandel	Avocado oil, refined	13361407	1
Caelo	Avocado oil, refined	13361414	6
Caelo	Avocado oil, refined	13361411	2
Caesar & Loretz GmbH Hi...	Avocado oil, refined	13361414	1
Caelo	Avocado oil, refined	13361441	1
Fagron	Avocado oil, refined	13J25-B03	1
Audor Pharma	Avocado oil, refined	13361414	1
Euro OTC	Avocado oil, refined	1402027-01	5
Euro OTC	Avocado oil, refined	1410027-01	1
Caelo	Avocado oil, refined	14170104	8
Raben-Apotheke Mildenau	Avocado oil, refined	1402027-01	1
Sanacorp	Avocado oil, refined	14170104	1
Caelo	Avocado oil, refined	14363702	7
Bombastus	Avocado oil, refined	1402027-01	1
Caelo	Avocado oil, refined	14363703	7
Caelo	Avocado oil, refined	14363706	2
Euro OTC	Avocado oil, refined	1501015-01	1
Caelo	Avocado oil, refined	15155207	2
Caelo	Avocado oil, refined	15268203	4
Euro OTC	Avocado oil, refined	28041506	1
Bombastus	Avocado oil, refined	289240	1
Caelo	Avocado oil, refined	19081501	1
Euro OTC	Avocado oil, refined	30121424	1
Bombastus	Avocado oil, refined	268579	1
Henry Lamotte Oils	Avocado oil, refined	122470	1
Caelo	Avocado oil, refined	3413M-01960	2
Henry Lamotte Oils GmbH	Avocado oil, refined	122490	2
Henry Lamotte Oils GmbH	Avocado oil, refined	130143	2
Lamotte	Avocado oil, refined	122490	1
Bombastus	Avocado oil, refined	286519	1
Caelo	Avocado oil, refined	130172	1
Lamotte/Sanacorp	Avocado oil, refined	130193	1
HenryLamotte/Phoenix	Avocado oil, refined	130143	1
Lamotte	Avocado oil, refined	130143	1
Henry Lamotte	Avocado oil, refined	130143	1
Bombastus	Avocado oil, refined	2091235000130	1
Caelo	Avocado oil, refined	2081303	1
PVL	Avocado oil, refined	2807133	1
PVL	Avocado oil, refined	2410131	1

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Supplier	Substance	Batch	Spectra
Caelo	Avocado oil, refined	11147607	1
Euro OTC	Avocado oil, refined	1112018-01	1
Caesar/Noweda	Avocado oil, refined	12064801	1
Caelo	Avocado oil, refined	11227207	2
Großhandel	Avocado oil, refined	12064801	1
Caelo	Avocado oil, refined	12064810	3
Anzag 16.10.12 ek: 3,90EUR	Avocado oil, refined	1204047-01	1
Caelo	Avocado oil, refined	12064802	2
Caelo	Avocado oil, refined	12064804	2
Caelo	Avocado oil, refined	12064813	3
Caesar/Noweda	Avocado oil, refined	12064812	2
Anzag 06.02.2013	Avocado oil, refined	1208028-01	1
Großhandel	Avocado oil, refined	12248302	1
Caelo	Avocado oil, refined	12248302	2
Caelo	Avocado oil, refined	12248303	2
Phoenix 30.04.2013	Avocado oil, refined	12248310	2
Caelo	Avocado oil, refined	12248310	11
Caesar & Loretz/ Noweda	Avocado oil, refined	12248312	3
Caelo	Avocado oil, refined	12248315	2
Fagron	Avocado oil, refined	12H24-N02	1
Euro OTC	Avocado oil, refined	1301039-01	1
Caesar & Loretz GmbH	Avocado oil, refined	12H24-N02	1
Caelo	Avocado oil, refined	13031303	1
Großhandel	Avocado oil, refined	13129102	1
Caelo	Avocado oil, refined	1304039-1	1
gehe 15.01.2014	Avocado oil, refined	1305046-01	1
Noveda	Avocado oil, refined	13129103	1
Caelo	Avocado oil, refined	13129104	2
Caelo	Avocado oil, refined	13129106	2
spinnrad	Avocado oil, refined	413301212	1
Bombastus	Avocado oil, refined	274935	1
spinnrad	Avocado oil, refined	212301211	1
Caelo	Avocado oil, refined	28111308	1
Taoasis	Avocado oil, refined	92010-105977	1
Phönix 15.01.2014	Avocado oil, refined	279025	1
Caelo	Avocado oil, refined	5216901	1
Caelo	Avocado oil, refined	4718201	2
Taoasis	Avocado oil, refined		1
EuRho	Avocado oil, refined	4111M-01960	1
Caelo	Almond oil, refined	2204130	1
Henry Lamotte Oils GmbH	Borage oil, refined, stabili...	130402	1
Spinnrad	Borage oil, refined, stabili...	1115204582	1
Lamotte/Alliance	Borage oil, refined, stabili...	125354	1
Caelo	Borage oil, refined, stabili...	13372104	6
Henry Lamotte	Borage oil, refined, stabili...	145579	1
Caelo	Borage oil, refined, stabili...	13170607	1
Caelo	Borage oil, refined, stabili...	13372106	2
Caelo	Borage oil, refined, stabili...	13372107	8
Caelo	Borage oil, refined, stabili...	14161901	4
Caelo	Borage oil, refined, stabili...	14161904	3
Caelo	Borage oil, refined, stabili...	14203001	3
Caelo	Borage oil, refined, stabili...	14161906	2
Caelo	Borage oil, refined, stabili...	1416906	1
Caelo	Borage oil, refined, stabili...	14203004	11
Phönix 14.01.15	Borage oil, refined, stabili...	14203004	1
Caelo	Borage oil, refined, stabili...	14203005	9
Sanacorp	Borage oil, refined, stabili...	14203006	1
Caelo	Borage oil, refined, stabili...	14203009	1
Caelo	Borage oil, refined, stabili...	14203011	4
Caelo	Borage oil, refined, stabili...	14203012	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Borage oil, refined, stabili...	14203012	1
Caelo	Borage oil, refined, stabili...	1461906	1
Caelo	Borage oil, refined, stabili...	15063401	2
Fagron	Borage oil, refined, stabili...	14A20-B03	1
Caelo	Borage oil, refined, stabili...	15063402	10
Caelo	Borage oil, refined, stabili...	15063407	8
Caelo	Borage oil, refined, stabili...	15063406	2
Euro OTC	Borage oil, refined, stabili...	15063407	1
Caelo	Borage oil, refined, stabili...	15063409	2
Caelo	Borage oil, refined, stabili...	15063408	3
Caelo	Borage oil, refined, stabili...	15063411	5
Caelo	Borage oil, refined, stabili...	15063412	1
Caelo	Borage oil, refined, stabili...	15063413	1
Caesar & Loretz GmbH / ...	Borage oil, refined, stabili...	15063412	1
Caelo	Borage oil, refined, stabili...	15305001	8
Caelo	Borage oil, refined, stabili...	26041404	1
Caelo	Borage oil, refined, stabili...	15305005	3
PG-Naturpharm	Borage oil, refined, stabili...	397-045	2
Caelo	Borage oil, refined, stabili...	15305003	4
Lamotte/Noweda	Borage oil, refined, stabili...	5404602	1
Caelo	Borage oil, refined, stabili...	15305009	4
Caelo	Borage oil, refined, stabili...	15305011	1
Caelo	Borage oil, refined, stabili...	16052302	1
	Borage oil, refined, stabili...	123387	1
Henry Lamotte GmbH Bremen	Borage oil, refined, stabili...	122791	1
Caelo	Borage oil, refined, stabili...	16052301	1
Caelo	Borage oil, refined, stabili...	11002607	1
Caelo	Borage oil, refined, stabili...	16266002	1
Caelo	Borage oil, refined, stabili...	123118	1
Caelo	Borage oil, refined, stabili...	11260102	2
Caelo	Borage oil, refined, stabili...	12027004	1
Caelo	Borage oil, refined, stabili...	11260106	2
Caelo	Borage oil, refined, stabili...	12152108	1
Caelo	Borage oil, refined, stabili...	12161202	8
Caelo	Borage oil, refined, stabili...	12027008	2
Gehe	Borage oil, refined, stabili...	12027008	1
Noweda	Borage oil, refined, stabili...	12027006	1
Noweda	Borage oil, refined, stabili...	12161202	2
Kehr	Borage oil, refined, stabili...	12161202	1
Caesar/Noweda	Borage oil, refined, stabili...	12161202	1
Gehe	Borage oil, refined, stabili...	12161203	1
Caelo	Borage oil, refined, stabili...	12161205	3
Caelo	Borage oil, refined, stabili...	12161203	1
Caelo	Borage oil, refined, stabili...	12161207	5
Caelo	Borage oil, refined, stabili...	1235504	1
Noweda	Borage oil, refined, stabili...	12355203	1
Caelo	Borage oil, refined, stabili...	12161209	1
Caelo	Borage oil, refined, stabili...	12355203	9
Phoenix	Borage oil, refined, stabili...	12355203	1
Caelo	Borage oil, refined, stabili...	12355205	4
Caesar/Noweda	Borage oil, refined, stabili...	13136501	1
Caelo	Borage oil, refined, stabili...	12365203	1
Caelo	Borage oil, refined, stabili...	1235523	1
J.H.Müller/direkt/17.05...	Borage oil, refined, stabili...	130302	1
Noweda	Borage oil, refined, stabili...	13136504	1
Caelo	Borage oil, refined, stabili...	13136504	10
Caesar/Noweda	Borage oil, refined, stabili...	13136504	1
Caelo	Borage oil, refined, stabili...	1316504	1
Caelo	Borage oil, refined, stabili...	13170601	4
Caelo	Borage oil, refined, stabili...	13170605	3

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Supplier	Substance	Batch	Spectra
Caelo	Borage oil, refined, stabili...	13170604	1
Caelo	Borage oil, refined, stabili...	13170606	17
Noweda	Borage oil, refined, stabili...	13170606	1
Caelo	Borage oil, refined, stabili...	13170610	6
	Borage oil, refined, stabili...	13170606	1
Caelo	Borage oil, refined, stabili...	13170613	4
Noweda	Borage oil, refined, stabili...	13372101	1
Caesar/Noweda	Borage oil, refined, stabili...	13372103	1
Noweda	Borage oil, refined, stabili...	13372104	1
Phoenix	Borage oil, refined, stabili...	14161906	1
Caelo	Borage oil, refined, stabili...	1713M-02881	1
Anzag 15.10.12	Borage oil, refined, stabili...	965-028	2
Henry Lamotte	Borage oil, refined, stabili...	5402901	3
Bergland-Pharma	Borage oil, refined, stabili...	H103019	2
Caelo	Oleyl oleate (stabilised)	10298401	2
Fagron	Oleyl oleate (stabilised)	11108-N03	1
Caelo	Oleyl oleate (stabilised)	12067701	1
Caelo	Oleyl oleate (stabilised)	12067704	7
Noweda	Oleyl oleate (stabilised)	15321706	1
Caelo	Oleyl oleate (stabilised)	11292610	1
Noweda	Oleyl oleate (stabilised)	12067704	3
Caelo	Oleyl oleate (stabilised)	12142803	1
Caelo	Oleyl oleate (stabilised)	12067705	2
Caelo	Oleyl oleate (stabilised)	12220201	1
Caelo	Oleyl oleate (stabilised)	12220205	4
Caelo	Oleyl oleate (stabilised)	12220204	1
VDL	Oleyl oleate (stabilised)	12220205	2
Caelo	Oleyl oleate (stabilised)	12220207	3
Gehe	Oleyl oleate (stabilised)	12220207	1
Caelo	Oleyl oleate (stabilised)	12220210	1
Caelo	Oleyl oleate (stabilised)	13167109	4
Caelo	Oleyl oleate (stabilised)	13096401	1
Caelo	Oleyl oleate (stabilised)	122220210	1
Caelo	Oleyl oleate (stabilised)	13096407	1
Caelo	Oleyl oleate (stabilised)	14005001	1
gehe 20.08.2013	Oleyl oleate (stabilised)	13167109	1
Caelo	Oleyl oleate (stabilised)	13291607	1
Caelo	Oleyl oleate (stabilised)	21061302	1
SysKem Chemie	Oleyl oleate (stabilised)	8002060413	1
Caelo	Oleyl oleate (stabilised)	26071210	1
SysKem Chemie	Oleyl oleate (stabilised)	35885	1
Caelo	Oleyl oleate (stabilised)		2
Caelo	Decyl oleate	15082206	3
Caelo	Decyl oleate	15191502	2
Caelo	Decyl oleate	15248405	6
Caelo	Decyl oleate	16107101	3
Sanacorp	Decyl oleate	13378403	1
Caelo	Decyl oleate	14005002	1
Caelo	Decyl oleate	14005001	2
Raben-Apotheke Mildenau	Decyl oleate	14814-B03-292195	1
Caelo	Decyl oleate	15082205	1
Sanacorp	Decyl oleate	15082206	1
Caelo	Decyl oleate	15191501	1
Caelo	Decyl oleate	13291606	2
Caelo	Decyl oleate	15047702	2
Euro OTC	Decyl oleate	1309018-01	1
Caelo	Decyl oleate	15393704	1
Fagron	Peanut oil, refined	133498	1
Fagron	Peanut oil, refined	1410-B07-300438	1
Fagron	Peanut oil, refined	14I10-B07-300438	2

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Supplier	Substance	Batch	Spectra
Caelo	Peanut oil, refined	15273402	7
Caelo	Peanut oil, refined	15331501	3
Caelo	Peanut oil, refined	15331503	4
Caelo	Peanut oil, refined	15331502	9
Caelo	Peanut oil, refined	15331506	1
Fagron	Peanut oil, refined	15E07-B04-308779	2
Caelo	Peanut oil, refined	16071101	8
Fagron	Peanut oil, refined	15B11B02304989	2
Caelo	Peanut oil, refined	16071102	8
Jenne	Peanut oil, refined	16071104	1
Caelo	Peanut oil, refined	16071105	8
Caelo	Peanut oil, refined	16071104	2
Caesar & Loretz/AHC	Peanut oil, refined	16071104	1
Caelo	Peanut oil, refined	16071106	2
Bombastus	Peanut oil, refined	295272	4
Caelo	Peanut oil, refined	16249502	2
Bombastus	Peanut oil, refined	299136	3
Bombastus	Peanut oil, refined	30100	1
Caelo	Peanut oil, refined	160711104	1
Bombastus	Peanut oil, refined	302017	2
Ebert & Jacobi 5.7.16	Peanut oil, refined	8000666005	3
Ebert KKH 20.09.16	Peanut oil, refined	8001417003	2
Caelo	Peanut oil, refined		3
Fagron	Peanut oil, refined	131943	1
Caelo	Peanut oil, refined	13173003	1
Caelo	Peanut oil, refined	13051403	1
Fagron	Peanut oil, refined	130723	1
Fagron	Peanut oil, refined	13306103	3
Caelo	Peanut oil, refined	13358801	10
Caelo	Peanut oil, refined	13358804	18
Fagron	Peanut oil, refined	13j25b06291837	1
Fagron	Peanut oil, refined	13J25-B06-291838	2
Caleo	Peanut oil, refined	14/10-B07	1
Fagron	Peanut oil, refined	14/10-B07-300426	1
Caelo	Peanut oil, refined	14033601	15
Caelo	Peanut oil, refined	14115403	5
Caelo	Peanut oil, refined	14115404	11
Cealo/Phoenix	Peanut oil, refined	14115405	1
Caelo	Peanut oil, refined	14246902	5
Caelo	Peanut oil, refined	14246903	12
Fagron	Peanut oil, refined	14246901	1
Caelo	Peanut oil, refined	1424693	1
Hedinger	Peanut oil, refined	14355903	1
Caelo	Peanut oil, refined	14355903	5
Fagron	Peanut oil, refined	14355904	2
Caelo	Peanut oil, refined	14355905	7
Fagron	Peanut oil, refined	14D11-B05-294677	4
Fagron	Peanut oil, refined	14D11-B05-294672	2
Fagron	Peanut oil, refined	14I-10B07-300438	1
Caelo	Peanut oil, refined	15015104	11
Caelo	Peanut oil, refined	15015106	3
caesar&loretz,phönix	Peanut oil, refined	1508506	1
Caelo	Peanut oil, refined	15208501	3
Caelo	Peanut oil, refined	15208505	13
Caelo	Peanut oil, refined	15208506	14
Caelo	Peanut oil, refined	15273403	7
Phönix Gotha	Peanut oil, refined	15273403	1
Caesar & Loretz GmbH Hi...	Peanut oil, refined	15331502	1
Fagron	Peanut oil, refined	15E07-B04	1
Cealo/AHD	Peanut oil, refined	16071101	1

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Supplier	Substance	Batch	Spectra
Caelo	Peanut oil, refined	20021502	1
Caelo	Peanut oil, refined	23051406	1
Caelo	Peanut oil, refined	25091405	1
Bombastus	Peanut oil, refined	286393	1
Bombastus	Peanut oil, refined	291671	1
Bombastus	Peanut oil, refined	288510	1
Caelo	Peanut oil, refined	30121415	1
Caelo	Peanut oil, refined	3614M-01954	1
lamotte/Gehe	Peanut oil, refined	5473601	2
Henry Lamotte	Peanut oil, refined	5204402	1
Henry Lamotte	Peanut oil, refined	5473601	1
Lamotte/Phoenix	Peanut oil, refined	5592601	1
lamotte/Gehe	Peanut oil, refined	5592601	3
Henry Lamotte oils GmbH...	Peanut oil, refined	5592601	2
lamotte/Phönix	Peanut oil, refined	5697901	1
Henry Lamotte	Peanut oil, refined	5699601	2
Henry Lamotte	Peanut oil, refined	5697901	2
Lamotte/Phoenix	Peanut oil, refined	5699601	2
Henry Lamotte oils GmbH...	Peanut oil, refined	5699601	2
Henry Lamotte	Peanut oil, refined	5904100001	2
Lamotte/Phoenix	Peanut oil, refined	5904100001	1
Bombastus	Peanut oil, refined	266753	1
Fagron	Peanut oil, refined	P101P102P103	1
Bombastus	Peanut oil, refined	267966	2
Bombastus	Peanut oil, refined	271512	3
Caelo	Peanut oil, refined	3061303	1
Caelo	Peanut oil, refined	6061202	1
Bombastus	Peanut oil, refined	8273799	1
Henry Lamotte	Peanut oil, refined	611Erdnuss	1
Caelo	Peanut oil, refined	9101201	1
Caelo	Peanut oil, refined	1013A-01954	2
Caelo	Peanut oil, refined	9091303	1
Caelo	Peanut oil, refined	7031307	1
Phönix Gotha	Peanut oil, refined	101453	1
Caelo	Peanut oil, refined	10208605	1
H.Lamotte/Noweda	Peanut oil, refined	1034	1
Caelo	Peanut oil, refined	10358602	1
Caelo	Peanut oil, refined	11100201	2
Caelo	Peanut oil, refined	11163201	1
Phönix Gotha	Peanut oil, refined	11163203	1
Caelo	Peanut oil, refined	11254503	1
Caelo	Peanut oil, refined	11254504	1
Caelo	Peanut oil, refined	11313905	4
Purren Apotheke	Peanut oil, refined	11313905	1
Caelo	Peanut oil, refined	11313906	3
EuRho	Peanut oil, refined	1204018-01	1
Caelo	Peanut oil, refined	12041902	12
Noweda	Peanut oil, refined	12041902	4
Anzag am 4.05.2012	Peanut oil, refined	12041902	2
Gehe	Peanut oil, refined	12041902	1
Caelo	Peanut oil, refined	1207211954	1
Caelo	Peanut oil, refined	12080802	1
Caelo	Peanut oil, refined	12101502	3
Caelo	Peanut oil, refined	12101503	10
Noweda	Peanut oil, refined	12101503	1
Caelo	Peanut oil, refined	12203803	18
Caelo	Peanut oil, refined	1211503	1
Erika apotheke	Peanut oil, refined	12203803	1
Noweda	Peanut oil, refined	12203803	1
Anzag 07.12.12	Peanut oil, refined	12203803	1

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Supplier	Substance	Batch	Spectra
Caelo	Peanut oil, refined	12274302	26
Caelo	Peanut oil, refined	12274032	1
Noweda	Peanut oil, refined	12274302	5
Großhandel	Peanut oil, refined	12274302	1
Phönix	Peanut oil, refined	12274302	2
Caelo	Peanut oil, refined	12323204	14
AHD, 06.05.2013	Peanut oil, refined	12323204	1
Anzag	Peanut oil, refined	12323204	1
Noweda	Peanut oil, refined	123508	1
Fagron	Peanut oil, refined	12A05-N05	1
Fagron	Peanut oil, refined	12C30-N02	2
Anzag	Peanut oil, refined	12c30n02	1
Fagron	Peanut oil, refined	12c30-n02	1
Noweda	Peanut oil, refined	12C30-N02	1
Phönix Gotha	Peanut oil, refined	12C30-N02	1
Fagron	Peanut oil, refined	12H31-N05	4
Anzag	Peanut oil, refined	12H31N05	1
Fagron	Peanut oil, refined	12J23-N01	3
Fagron	Peanut oil, refined	12J23-N01	1
Fagron	Peanut oil, refined	13G30-N05	1
Caelo	Peanut oil, refined	13129202	1
Caelo	Peanut oil, refined	13129203	35
Phönix Gotha	Peanut oil, refined	13129202	1
Alliance Healthcare	Peanut oil, refined	13129203	1
Großhandel	Peanut oil, refined	13129203	1
Caelo	Peanut oil, refined	13306101	2
Gehe	Peanut oil, refined	13306103	1
Phönix Gotha	Peanut oil, refined	13306103	1
Caelo	Peanut oil, refined	13306106	16
Gehe	Peanut oil, refined	13306106	1
Phoenix	Peanut oil, refined	13306106	1
Phoenix	Peanut oil, refined	13358803	1
Caelo	Peanut oil, refined	1335884	1
Caelo	Peanut oil, refined	1358804	1
Fagron	Peanut oil, refined	13g30-n05	1
Fagron	Peanut oil, refined	13J25B06291837	1
Caesar&lorenz,Phoenix	Peanut oil, refined	14033601	1
Caelo	Peanut oil, refined	15012016	1
Caesar&lorenz,Phoenix	Peanut oil, refined	14246903	1
Caelo	Peanut oil, refined	24081208	1
Bombastus	Peanut oil, refined	276103	1
Bombastus	Peanut oil, refined	277813	1
Caelo	Peanut oil, refined	26061203	1
Caelo	Peanut oil, refined	21121205	1
Caelo	Peanut oil, refined	30101312	1
Caelo	Peanut oil, refined	3813E1954	1
Noweda	Peanut oil, refined	5103001	1
Caelo	Peanut oil, refined	3112M-01954	1
Fagron	Peanut oil, refined	5012A-01954	1
Anzag 16.01.13 ek.5.13	Peanut oil, refined	5204402	2
Lamotte/GEHE	Peanut oil, refined	5204402	2
Phönix	Peanut oil, refined	5204402	1
Caelo	Peanut oil, refined	5204402	1
Henry Lamotte oils GmbH	Peanut oil, refined	5204402	2
Lamotte	Peanut oil, refined	5204402	2
Henry Lamotte/Jenne	Peanut oil, refined	5204402	1
Henry Lamotte	Peanut oil, refined	520442	1
Fiebig 02.10.12 ek: 5,13EUR	Peanut oil, refined	5231601	1
H.Lamotte/Noweda	Peanut oil, refined	5231601	1
Phönix	Peanut oil, refined	5404101	1

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Supplier	Substance	Batch	Spectra
HenryLamotte/Phoenix	Peanut oil, refined	5231601	1
lamotte/Jenne	Peanut oil, refined	5404101	1
Lamotte / Gehe	Peanut oil, refined	5404101	1
Phönix	Peanut oil, refined	5473601	1
H.Lamotte/Noweda	Peanut oil, refined	5473601	1
Bombastus	Peanut oil, refined	80370408	1
Caelo	Peanut oil, refined	ch12274302	1
H.Lamotte/Noweda	Peanut oil, refined	5699601	1
Henry Lamotte	Peanut oil, refined	5592601	1
Euro OTC	Soy lecithin, liquid	1503038-02	1
Caelo	Codliver oil (type A)	14305701	1
Caelo	Codliver oil (type A)	13396403	2
Caelo	Codliver oil (type A)	15047201	6
Henry Lamotte Oils	Codliver oil (type A)	5529601	2
Lamotte/Stumpf	Codliver oil (type A)	5529601	1
Caelo	Codliver oil (type A)	5693101	2
Caelo	Codliver oil (type A)	12346810	8
henry lamotte oils	Codliver oil (type A)	5437202	1
Henry Lamotte Oils	Codliver oil (type A)	5693101	1
Caelo	Codliver oil (type A)	13106201-3392131070	1
Caelo	Codliver oil (type A)	5437202	12
Taoasis	Jojoba oil, native	137640-123934	1
Caelo	Jojoba oil, native	15116903	2
Taoasis	Jojoba oil, native	133535-123399	1
Caelo	Jojoba oil, native	15409903	2
Taoasis	Jojoba oil, native	151214-125861	2
Caelo	Jojoba oil, native	15116904	2
Caelo	Jojoba oil, native	15409904	1
Bombastus	Jojoba oil, native	294112	3
Caelo	Jojoba oil, native	16070602	1
Sanacorp	Jojoba oil, native	5756401	3
Primavera	Jojoba oil, native	241H23	1
Henry Lamotte Oils GmbH	Jojoba oil, native	5913600001	2
Taoasis	Jojoba oil, native	133535-123190	2
Caelo	Jojoba oil, native	14052201	1
Caelo	Jojoba oil, native	14284202	4
Caelo	Jojoba oil, native	14284203	2
Caelo	Jojoba oil, native	14284204	4
Caelo	Jojoba oil, native	14284208	2
Caelo	Jojoba oil, native	21041504	1
Taoasis	Jojoba oil, native	2A5890402-121152	2
Henry Lamotte	Jojoba oil, native	5404201	1
Spinnrad	Jojoba oil, native	315601031	1
Lamotte	Jojoba oil, native	5732801	1
Henry Lamotte/Alliance ...	Jojoba oil, native	5756401	1
Henry Lamotte / AHD	Jojoba oil, native	5756401	1
Caelo	Jojoba oil, native	3071301	1
DAC 2006	Jojoba oil, native	11358102	1
Caelo	Jojoba oil, native	10071307	1
Caelo	Jojoba oil, native	11078605	2
Caelo	Jojoba oil, native	11358102	1
Caelo	Jojoba oil, native	11358103	1
Caelo	Jojoba oil, native	12114701	1
Caelo	Jojoba oil, native	12114702	1
Caelo	Jojoba oil, native	12114708	1
Caelo	Jojoba oil, native	12217003	1
Caelo	Jojoba oil, native	12114703	1
Großhandel	Jojoba oil, native	12217004	1
Caelo	Jojoba oil, native	12217008	2
Caelo	Jojoba oil, native	12217009	3

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Supplier	Substance	Batch	Spectra
Caelo	Jojoba oil, native	12217010	5
Caelo	Jojoba oil, native	13011202	5
Gehe Laborchemie Apolda...	Jojoba oil, native	13011202	1
Caelo	Jojoba oil, native	13011203	4
Caelo	Jojoba oil, native	13011204	4
Caelo	Jojoba oil, native	13129001	3
Caelo	Jojoba oil, native	13129004	5
Caelo	Jojoba oil, native	13129005	2
Caelo	Jojoba oil, native	13129006	5
Großhandel	Jojoba oil, native	13129006	1
Caelo	Jojoba oil, native	13287701	2
Primavera	Jojoba oil, native	17009133	1
Caelo	Jojoba oil, native	15011412	1
Caelo	Jojoba oil, native	17121302	1
Primavera	Jojoba oil, native	19307131	1
Caelo	Jojoba oil, native	19061307	1
Caelo	Jojoba oil, native	25101303	1
wilco	Jojoba oil, native	2480	1
Caelo	Jojoba oil, native	2613M-01986	1
Bombastus	Jojoba oil, native	276323	1
Taoasis	Jojoba oil, native	4674401-67053	1
HenryLamotte	Jojoba oil, native	4957101	1
Anzag/	Jojoba oil, native	5115601	1
HenryLamotte	Jojoba oil, native	5172601	9
Lamotte/Gehe	Jojoba oil, native	5172601	1
Anzag	Jojoba oil, native	5172601	1
Henry Lamotte	Jojoba oil, native	5194301	1
Taoasis	Jojoba oil, native	5225101-108329	1
Taoasis	Jojoba oil, native	5336301-111368	1
HenryLamotte	Jojoba oil, native	5194301	1
Lamotte/Sanacorp	Jojoba oil, native	5194301	1
Taoasis	Jojoba oil, native	5336301-109515	1
Taoasis	Jojoba oil, native	5406801-111216	1
Taoasis	Jojoba oil, native	5406801-111877	1
Henry Lamotte	Jojoba oil, native	5429201	3
Taoasis	Jojoba oil, native	5445301-112580	2
Taoasis GmbH	Jojoba oil, native	5445301-112580	1
Bombastus	Jojoba oil, native	281299	1
H. Lamotte/Noweda	Codliver oil (type A)	119929	2
Gehe/Henry Lamotte Oils...	Codliver oil (type A)	119929	1
Henry Lamotte	Codliver oil (type A)	119929	1
Henry Lamotte Oils GmbH...	Codliver oil (type A)	123823	1
Henry Lamotte Oils GmbH	Codliver oil (type A)	123420L900	1
Lamotte/V.d.L.	Codliver oil (type A)	123823	1
Caelo	Codliver oil (type A)	3121201	1
Caelo	Codliver oil (type A)	3021402	1
Henry Lamotte Oils	Codliver oil (type A)	2101204	1
Caelo	Codliver oil (type A)	5091309	1
Caelo	Codliver oil (type A)	11081202	1
Caelo	Codliver oil (type A)	10061302	1
Caelo	Codliver oil (type A)	5061202	1
Caelo	Codliver oil (type A)	6021302	1
Caelo	Codliver oil (type A)	10101207	1
Caelo	Codliver oil (type A)	11315302	2
Caelo	Codliver oil (type A)	12009301	1
Caelo	Codliver oil (type A)	12009302	5
Caelo	Codliver oil (type A)	11315303	1
Caelo	Codliver oil (type A)	12009308	2
Caelo	Codliver oil (type A)	12062501	9
Anzag 17.12.2012	Codliver oil (type A)	12062501	1

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Supplier	Substance	Batch	Spectra
Großhandel	Codliver oil (type A)	12062501	1
Caelo	Codliver oil (type A)	12126102	1
Caelo	Codliver oil (type A)	12148703	11
Caelo	Codliver oil (type A)	121487703	1
Caelo	Codliver oil (type A)	13065503	4
Caelo	Codliver oil (type A)	13069201	2
Caelo	Codliver oil (type A)	13011301	1
Großhandel	Codliver oil (type A)	13106201	1
Alliance Health 21.10.2...	Codliver oil (type A)	13106201	2
Caelo	Codliver oil (type A)	13277706	8
Großhandel	Codliver oil (type A)	13277706	1
Caelo	Codliver oil (type A)	14061312	1
Caelo	Codliver oil (type A)	18031308	1
Henry Lamotte	Codliver oil (type A)	20021413	1
Henry Lamotte	Codliver oil (type A)	18101303	1
Caelo	Codliver oil (type A)	21111204	1
Caelo	Codliver oil (type A)	25091210	1
Caelo	Codliver oil (type A)	26061202	1
Henry Lamotte	Codliver oil (type A)	26111303	1
Caelo	Codliver oil (type A)	30041302	1
lamotte	Codliver oil (type A)	5029205	1
Henry Lamotte	Codliver oil (type A)	30041303	1
Henry Lamotte Oils GmbH	Codliver oil (type A)	5029207	1
Henry Lamotte	Codliver oil (type A)	5029207	1
Henry Lamotte Oils GmbH	Codliver oil (type A)	5228001	3
Henry Lamotte	Codliver oil (type A)	5228001	1
Henry Lamotte Oils	Codliver oil (type A)	5228001	1
H.Lamotte/Noweda	Codliver oil (type A)	5228001	1
Lamotte Jenne	Codliver oil (type A)	5228004	2
H.Lamotte/Noweda	Codliver oil (type A)	5228004	1
Henry Lamotte	Codliver oil (type A)	5228004	1
Henry Lamotte GmbH	Codliver oil (type A)	5228004	1
Henry Lamotte GmbH	Codliver oil (type A)	5437202	1
Hustadt Apotheke	Codliver oil (type A)	5437202	1
Lamotte/ Noweda	Codliver oil (type A)	5437202	7
Dr. Paulsen	Codliver oil (type A)	5437202	1
BREMER SCHLÜSSEL/ Noweda	Codliver oil (type A)	5437202	1
Gehe	Codliver oil (type A)	5437202	1
Henry Lamotte	Codliver oil (type A)	5437202	1
Henry Lamotte/V.d.L.	Codliver oil (type A)	5437202	1
Henry Lamotte	Codliver oil (type A)	5529601	6
Caelo	Codliver oil (type A)	5529601	6
Henry Lamotte/Phoenix	Codliver oil (type A)	5529601	2
Bremen / Noweda	Codliver oil (type A)	5529601	1
Lamotte/Noweda	Codliver oil (type A)	5529601	1
henry lamotte	Codliver oil (type A)	5529601	1
Lamotte/ Noweda	Codliver oil (type A)	A458	2
Lamotte/V.d.L.	Codliver oil (type A)	5529601	4
Caelo	Codliver oil (type A)	2121404	1
Caelo	Codliver oil (type A)	10031501	1
Caelo	Codliver oil (type A)	5081402	1
Caelo	Codliver oil (type A)	4061403	1
Caelo	Codliver oil (type A)	10061501	1
Caelo	Codliver oil (type A)	8071504	1
Caelo	Codliver oil (type A)	13106201	8
Caelo	Codliver oil (type A)	13277707	1
Caelo	Codliver oil (type A)	13396407	4
Caelo	Codliver oil (type A)	14075015	1
Caelo	Codliver oil (type A)	14305003	1
Caelo	Codliver oil (type A)	15201203	2

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Supplier	Substance	Batch	Spectra
Caelo	Codliver oil (type A)	15201201	1
Caelo	Codliver oil (type A)	15325201	2
Caesar & Loretz/Noweda	Codliver oil (type A)	15325201	1
Caelo	Codliver oil (type A)	16018202	1
Großhandel	Codliver oil (type A)	196403	1
Caelo	Codliver oil (type A)	17011503	1
Caelo	Codliver oil (type A)	21101401	1
Caelo	Codliver oil (type A)	23121414	1
Henry Lamotte	Codliver oil (type A)	26111402	1
Caelo	Codliver oil (type A)	28071504	1
lamotte/Gehe	Codliver oil (type A)	5529601	4
pHOENIX 18.02.2014	Codliver oil (type A)	5529601	1
Caelo	Codliver oil (type A)	28041507	1
Henry Lamotte/Noweda	Codliver oil (type A)	5529601	1
Henry Lamotte oils GmbH...	Codliver oil (type A)	5529601	3
Fagron	Codliver oil (type A)	5529601	4
Noweda	Codliver oil (type A)	5529601	4
Noweda/Henry Lamotte	Codliver oil (type A)	5529601	2
lamotte/Gehe	Codliver oil (type A)	5641901	3
Henry Lamotte Oils GmbH...	Codliver oil (type A)	5641901	1
Lamotte über Sanacorp	Codliver oil (type A)	5641901	1
Henry Lamotte/Noweda	Codliver oil (type A)	5641901	1
Henry Lamotte Oils GmbH	Codliver oil (type A)	5641901	1
Henry Lamotte oils GmbH...	Codliver oil (type A)	5641901	1
Lamotte/gehe	Codliver oil (type A)	5693101	2
Henry Lamotte Oils/GEHE	Codliver oil (type A)	5693101	1
Stumpf/Henry Lamotte	Codliver oil (type A)	5693101	1
Lamotte / Gehe	Codliver oil (type A)	5693101	1
Lamotte	Codliver oil (type A)	5878701	3
Henry Lamotte Oils GmbH	Codliver oil (type A)	5693101	1
henry lamotte	Codliver oil (type A)	5693101	1
Stumpf / Hedinger	Codliver oil (type A)	5878701	1
Henry Lamotte Oils/Noweda	Codliver oil (type A)	5878701	1
Henry Lamotte	Codliver oil (type A)	8000601001	4
Caelo	Codliver oil (type A)	8000601001	1
Henry Lamotte Oils GmbH	Codliver oil (type A)	8000601001	2
lamotte jenne	Codliver oil (type A)	8000601001	1
Caelo	Codliver oil (type A)	8000918001	5
Noweda/Henry Lamotte	Codliver oil (type A)	8000601001	2
Lamotte/Geibo	Codliver oil (type A)	8000918001	2
Henry Lamotte Oils GmbH	Codliver oil (type A)	8000918001	1
Lamotte/Gehe	Codliver oil (type A)	8001176004	1
Lamotte	Codliver oil (type A)	8001176004	1
Caelo	Codliver oil (type A)	8001215002	4
Henry Lamotte	Codliver oil (type A)	8001215002	2
LaMotte/Spangro	Codliver oil (type A)	80117604	1
Phönix/Lamotte	Codliver oil (type A)		1
Lamotte	Codliver oil (type A)	119929	2
Synopharm am 10.09.2012	Codliver oil (type A)	119929	1
Henry Lamotte Oils, Anzag	Codliver oil (type A)	123823	2
Henry Lamotte Oils GmbH	Codliver oil (type A)	123108	1
Stumpf/Henry Lamotte	Codliver oil (type A)	119929	1
Caelo	Codliver oil (type A)	119929	1
Henry Lamotte oils GmbH	Codliver oil (type A)	123823	3
Lamotte/Phönix	Codliver oil (type A)	123823	1
Henry Lamotte/Sanacorp	Codliver oil (type A)	123823	1
Lamotte/L3	Codliver oil (type A)	123823	1
Stumpf/Henry Lamotte	Codliver oil (type A)	123823	1
lamotte/Gehe	Codliver oil (type A)	123823	1
Caelo	Codliver oil (type A)	8131-01985	1

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Supplier	Substance	Batch	Spectra
Phoenix	Codliver oil (type A)	11315303	1
Fagron	Codliver oil (type A)	12H15-N02	1
Caelo	Codliver oil (type A)	13347501	1
Gehe	Codliver oil (type A)	2613A-01985	1
Noweda	Codliver oil (type A)	4537202	1
Henry Lamotte Oils GmbH	Codliver oil (type A)	4931805	1
Henry Lamotte Oils GmbH	Codliver oil (type A)	5029205	3
Lamotte/ Sanacorp	Codliver oil (type A)	5029207	1
Noweda/Lamotte Oils	Codliver oil (type A)	5029207	1
Caelo	Codliver oil (type A)	5228001	1
Noweda	Codliver oil (type A)	5228001	1
Henry Lamotte Oils GmbH	Codliver oil (type A)	5228004	2
Klenk	Codliver oil (type A)	5228004	2
Lamotte	Codliver oil (type A)	5228004	1
Lamotte Oils GmbH / G	Codliver oil (type A)	5228004	1
Noweda / Henry Lamotte	Codliver oil (type A)	5437202	1
Lamotte/GEHE	Codliver oil (type A)	5437202	8
Henry Lamotte Oils GmbH	Codliver oil (type A)	5437202	3
Lamotte/gehe	Codliver oil (type A)	5437202	4
Lamotte Oils GmbH / E	Codliver oil (type A)	5437202	2
Lamotte	Codliver oil (type A)	5437202	4
Henry Lamotte/Sanacorp	Codliver oil (type A)	5529601	1
Henry Lamotte/Kehr	Codliver oil (type A)	5529601	1
Henry Lamotte Oils GmbH	Codliver oil (type A)	5529601	1
Hedinger	Codliver oil (type A)	8000601001	1
Henry Lamotte Oils, Gehe	Codliver oil (type A)	5529601	1
Henry Lamotte Oils/Noweda	Codliver oil (type A)	5529601	1
henry lamotte oils gmbh	Codliver oil (type A)	8000918001	1
henry lamotte oils gmbh	Codliver oil (type A)	8001176004	1
EUro/AHD	Soy lecithin, liquid	1305019-01	1
Henry/Jenne	Flaxseed oil, native	103277	3
Gehe	Soy lecithin, liquid	21022111/2	1
Henry/AHD	Flaxseed oil, native	124337	2
Euro OTC	Flaxseed oil, native	124116	1
Caelo	Flaxseed oil, native	14087903	1
Caelo	Flaxseed oil, native	13361202	4
Bombastus	Flaxseed oil, native	14087903	1
Lamotte	Flaxseed oil, native	124116	2
Caelo	Flaxseed oil, native	14087908	3
Caelo	Flaxseed oil, native	14087909	1
Caelo	Flaxseed oil, native	14306811	2
Caelo	Flaxseed oil, native	15116702	3
Caelo	Flaxseed oil, native	15175608	1
Bombastus	Flaxseed oil, native	285121	1
Gehe	Flaxseed oil, native	288025	1
Caesar & Loretz GmbH Hi...	Flaxseed oil, native	289164	1
Bombastus	Flaxseed oil, native	293950	1
statfold	Flaxseed oil, native	29409	1
Bombastus	Flaxseed oil, native	291126	1
Bombastus	Flaxseed oil, native	297286	1
statfold	Flaxseed oil, native	33588	2
Gehe/Vitalhaus	Flaxseed oil, native	160702	1
Bombastus	Flaxseed oil, native	296730	1
Lamotte/Otto	Flaxseed oil, native	5757301	1
Bombastus	Flaxseed oil, native	303096	1
Bombastus	Flaxseed oil, native	271645	2
Bombastus	Flaxseed oil, native	266111	1
Gehe	Flaxseed oil, native	273676	1
Bombastus	Flaxseed oil, native	272528	1
Kriger/Lamotte/30.12.13	Flaxseed oil, native	102503	1

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Supplier	Substance	Batch	Spectra
Noweda / Henry Lamotte	Flaxseed oil, native	119677	2
Noweda / Henry Lamotte	Flaxseed oil, native	119529	1
Phönix 11.09.2012	Flaxseed oil, native	118553	1
Stumpf/Henry Lamotte	Flaxseed oil, native	124116	1
Caelo	Flaxseed oil, native	7111204	1
Caelo	Flaxseed oil, native		2
Gehe	Flaxseed oil, native	12041701	1
Caelo	Flaxseed oil, native	12217504	2
Caelo	Flaxseed oil, native	12041701	1
Caelo	Flaxseed oil, native	12217505	2
Caelo	Flaxseed oil, native	13178203	3
Caelo	Flaxseed oil, native	12274205	2
Gehe	Flaxseed oil, native	13178203	1
Caelo	Flaxseed oil, native	13178209	1
Henry Lamotte Oils GMBH...	Flaxseed oil, native	12D05-N02	1
Caelo	Flaxseed oil, native	23021302	1
Bombastus	Flaxseed oil, native	275487	2
Bombastus	Flaxseed oil, native	276105	1
Bombastus	Flaxseed oil, native	276106	1
Bombastus	Flaxseed oil, native	276727	1
Bombastus	Flaxseed oil, native	279769	1
Bombastus	Flaxseed oil, native	280711	1
Bombastus	Flaxseed oil, native	281489	2
s.Prüfprotokoll	Flaxseed oil, native		1
Bombastus	Flaxseed oil, native	282391	1
Bombastus	Flaxseed oil, native	274875	1
Bomb/ Noweda	Flaxseed oil, native	290569	1
Caelo	Laurel oil	14176301	2
Caelo	Laurel oil	14176303	1
Caesar & Loretz/Noweda	Laurel oil	15216401	1
Caelo	Macadamia oil, refined	13012106	1
Caelo	Macadamia oil, refined	14179304	2
Caelo	Corn oil, refined	15296407	2
Caelo	Corn oil, refined	11267907	1
Caelo	Corn oil, refined	13010707	2
Caelo	Corn oil, refined	13010710	1
Henry Lamotte/Anzag	Almond oil, refined	416E-01950	1
Henry Lamotte/Gehe	Almond oil, refined	1000003242	1
Henry Lamotte Oils GmbH	Almond oil, refined	1000003242	2
Caelo	Almond oil, refined	15197401	7
Fagron	Almond oil, refined	15197404	1
Fagron	Almond oil, refined	12345	1
Caelo	Almond oil, refined	15197403	4
Caelo	Almond oil, refined	15197404	4
Caelo	Almond oil, refined	15197406	4
Caelo	Almond oil, refined	15409701	3
Caelo	Almond oil, refined	15197409	1
Caelo	Almond oil, refined	15409704	6
Caelo	Almond oil, refined	15409710	8
Alliance H.	Almond oil, refined	15409704	1
Caelo	Almond oil, refined	15409705	2
Caeolo/Noweda	Almond oil, refined	15409703	1
Caelo	Almond oil, refined	15409703	3
Phönix	Almond oil, refined	15409710	1
Fagron	Almond oil, refined	15409705	1
Caelo	Almond oil, refined	15409713	3
Caelo	Almond oil, refined	15409714	1
Euro OTC	Almond oil, refined	1603025-01	1
Caelo	Almond oil, refined	16071006	3
Caelo	Almond oil, refined	16071007	3

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Supplier	Substance	Batch	Spectra
Euro OTC	Almond oil, refined	16071002	1
Caelo	Almond oil, refined	16071002	3
Caelo	Almond oil, refined	16071008	1
Caelo	Almond oil, refined	16071003	1
Caelo	Almond oil, refined	16071009	1
Bombastus	Almond oil, refined	291509	3
Caelo	Almond oil, refined	1633327302	1
Bombastus	Almond oil, refined	298745	1
Taoasis	Almond oil, refined	33489-124674	1
Taoasis	Almond oil, refined	34371-125478	1
Bombastus	Almond oil, refined	302211	1
Henry Lamotte Oils GmbH	Almond oil, refined	8000725001	3
Lamotte/Phoenix	Almond oil, refined	8000712001	4
Bombastus	Almond oil, refined	302210	1
Taoasis	Almond oil, refined	31952-123336	1
Caelo	Almond oil, refined	8000915001	4
Henry Lamotte / Allianc...	Almond oil, refined	8000915001	2
Lamotte über Sanacorp	Almond oil, refined	8000915001	3
Noweda/Lamotte	Almond oil, refined	8000915001	1
henry lamotte oils Gmh/N	Almond oil, refined	8000915001	2
Lamotte	Almond oil, refined	8000915001	2
Henry Lamotte Oils GmbH	Almond oil, refined	8000915001	1
Henry Lamotte/ Noweda	Almond oil, refined	8000915001	2
Lamotte über Sanacorp	Almond oil, refined	8000915002	1
Henry Lamotte Olis GmbH	Almond oil, refined	8000915002	2
Caelo	Almond oil, refined	8000915002	2
Primavera	Almond oil, refined	11G23	2
Primavera	Almond oil, refined	82B23	2
henry lamotte oils Gmh/N	Almond oil, refined	8000915002	1
Henry Lamotte Sanacorp	Almond oil, refined	8001497001	1
Primavera	Almond oil, refined	218D24	1
Primavera	Almond oil, refined	21D24	1
Primavera	Almond oil, refined	480K23	1
Caelo	Almond oil, refined	465940	1
Taoasis	Almond oil, refined	12842-116104	1
Kehr / Lamotte	Almond oil, refined	50115PML01	1
Euro OTC	Almond oil, refined	540014-01	1
Caelo	Almond oil, refined	8041501	1
Eigenherstellung	Almond oil, refined	50115PML02	1
Eigenherstellung	Almond oil, refined	20915HML01	1
Caelo	Almond oil, refined	40315PML01	1
Caesar & Loretz GmbH Hi...	Almond oil, refined	510014-01	1
Eig	Almond oil, refined	80515HML01	1
Lamotte/AHD	Almond oil, refined	1000003242	2
Caelo	Almond oil, refined	10061502	1
Eigenherstellung	Almond oil, refined	120914HAS01	1
Caelo	Almond oil, refined	123test	1
Eigenherstellung	Almond oil, refined	120814HAS01	1
Taoasis	Almond oil, refined	130973-118607	1
Taoasis	Almond oil, refined	130973-116149	1
Euro OTC	Almond oil, refined	1310022-01	1
Euro OTC	Almond oil, refined	131002202	1
Aliance Hearthcave 11.0...	Almond oil, refined	13236402	1
Taoasis	Almond oil, refined	132805-118635	1
Caelo	Almond oil, refined	13236411	7
Fagron	Almond oil, refined	13350001	2
Caelo	Almond oil, refined	13326411	1
Caelo	Almond oil, refined	13350002	11
Ph.Eur.7.0	Almond oil, refined	13350003	1
Caelo	Almond oil, refined	13350006	7

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Supplier	Substance	Batch	Spectra
Caelo	Almond oil, refined	13350007	2
Taoasis	Almond oil, refined	134032-120671	1
Taoasis	Almond oil, refined	133805-120282	1
Taoasis	Almond oil, refined	134475-1215919	1
Taoasis	Almond oil, refined	135831-121621	2
Fagron	Almond oil, refined	13K28-B01-288270	1
Cealo/ Noweda	Almond oil, refined	14042704	1
Caelo	Almond oil, refined	14042702	2
Caelo	Almond oil, refined	1350003	1
Caelo	Almond oil, refined	14042704	2
Caelo	Almond oil, refined	14042705	7
Caelo	Almond oil, refined	14042706	5
Bombastus	Almond oil, refined	14042706	1
Caelo	Almond oil, refined	14042707	5
Caelo	Almond oil, refined	14042708	7
Caelo	Almond oil, refined	14042717	2
Caelo	Almond oil, refined	14042714	1
Euro OTC	Almond oil, refined	1407050-02	2
Euro OTC	Almond oil, refined	1407050-01	1
Caelo	Almond oil, refined	14139206	1
Caelo	Almond oil, refined	14139304	1
AHD	Almond oil, refined	14139305	1
Caelo	Almond oil, refined	14139306	2
Caelo	Almond oil, refined	14139309	2
Apolda/ Sanacorp	Almond oil, refined	14139309	1
Caelo	Almond oil, refined	1421508	1
Sanacorp	Almond oil, refined	1413935	1
Caesar & Loretz GmbH	Almond oil, refined	14215804	1
Caelo	Almond oil, refined	14215804	2
Caelo	Almond oil, refined	14215805	7
Caelo	Almond oil, refined	14215808	6
Apolda/ Sanacorp	Almond oil, refined	14215807	1
Gehe 22.12.14	Almond oil, refined	14215808	1
Fagron	Almond oil, refined	14215808	1
Caelo	Almond oil, refined	14215809	7
Gehe Kassel	Almond oil, refined	14215814	1
Caelo	Almond oil, refined	14215814	3
Caelo	Almond oil, refined	14215815	2
Caelo	Almond oil, refined	14215817	3
Caelo	Almond oil, refined	1439310	1
Fagron	Almond oil, refined	14D24-B07-296709	2
Fagron	Almond oil, refined	14F04-B01	1
Fagron	Almond oil, refined	14F04-B01-294721	2
Caelo	Almond oil, refined	15071406	1
Sanacorp	Almond oil, refined	15078401	1
Caelo	Almond oil, refined	15078402	4
Caelo	Almond oil, refined	15078403	6
GEHE 11.05.	Almond oil, refined	15078404	1
Caelo	Almond oil, refined	15078406	3
Caelo	Almond oil, refined	15078405	5
Euro	Almond oil, refined	1510014-01	1
Caelo	Almond oil, refined	15127302	2
Caelo	Almond oil, refined	15078407	2
Fagron	Almond oil, refined	15127303	1
Caelo	Almond oil, refined	15127304	3
Caelo	Almond oil, refined	15127305	4
Caelo	Almond oil, refined	15127306	7
Caelo	Almond oil, refined	15127307	3
Caelo	Almond oil, refined	15197402	6
Caelo	Almond oil, refined	15197407	7

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Supplier	Substance	Batch	Spectra
Caelo	Almond oil, refined	15197408	4
Caelo	Almond oil, refined	15409702	2
Caelo	Almond oil, refined	15409706	1
Fagron	Almond oil, refined	15F04-B01-309291	1
Fagron	Almond oil, refined	15F04-B01	1
Caelo	Almond oil, refined	18081402	1
Caelo	Almond oil, refined	17061403	1
Caelo	Almond oil, refined	16021510	1
Henry Lamotte Oils GmBH	Almond oil, refined	17082015B	1
Eigenherstellung	Almond oil, refined	180815HJK01	1
Caelo	Almond oil, refined	17111402	1
Eigenherstellung	Almond oil, refined	180915HML01	1
Caelo	Almond oil, refined	220515PML01	1
Bombastus	Almond oil, refined	283801	2
Eigenherstellung	Almond oil, refined	260515HML01	1
Bombastus	Almond oil, refined	284967	2
Caelo	Almond oil, refined	230315HML01	1
Bombastus	Almond oil, refined	286254	4
Bombastus	Almond oil, refined	284968	2
Caelo	Almond oil, refined	284968	1
Bombastus	Almond oil, refined	288428	1
Bombastus	Almond oil, refined	289709	1
Bombastus	Almond oil, refined	290136	1
Eigenherstellung	Almond oil, refined	290714HJK01	1
Eigenherstellung	Almond oil, refined	290714HJK02	1
Bombastus	Almond oil, refined	296519	1
Bombastus	Almond oil, refined	294784	2
Bombastus	Almond oil, refined	292591	1
Caelo	Almond oil, refined	29081404	1
Caelo	Almond oil, refined	30121416	1
Caelo	Almond oil, refined	31031403	1
Bombastus	Almond oil, refined	47/2014	1
Henry Lamotte Oils GmbH	Almond oil, refined	5415901	2
Bombastus	Almond oil, refined	5415901	3
Henry Lamotte / Noweda	Almond oil, refined	5415901	1
Caelo	Almond oil, refined	5415901	6
Henry Lamotte Oils GmbH...	Almond oil, refined	5415901	1
Henry Lamotte Oils	Almond oil, refined	5415901	2
Lamotte/Gehe	Almond oil, refined	5415901	6
Großhandel	Almond oil, refined	5415901	2
Henry Lamotte/Phoenix	Almond oil, refined	5615001	2
Gehe/Henry Lamotte Oils...	Almond oil, refined	5615001	2
Lamotte	Almond oil, refined	561001	1
Lamotte	Almond oil, refined	5415901	6
Lamotte / Alliance Heal...	Almond oil, refined	5615001	2
Phönix/ Lamotte	Almond oil, refined	5615001	1
Lamotte / Gehe	Almond oil, refined	5615001	1
Henry Lamotte Oils GmbH...	Almond oil, refined	5615001	1
lamotte/Gehe	Almond oil, refined	5615001	1
Lamotte/ Noweda	Almond oil, refined	5615001	3
Henry Lamotte	Almond oil, refined	5615001	4
Lamotte / Noweda	Almond oil, refined	5615001	1
Lamotte/Phönix	Almond oil, refined	5615003	1
Henry Lamotte Oils GmbH...	Almond oil, refined	5615001	1
LAMOTTE/NOWEDA	Almond oil, refined	5615003	4
Phönix/ Lamotte	Almond oil, refined	5615003	2
Lamotte/Phoenix	Almond oil, refined	5615003	2
Noweda/Henry Lamotte	Almond oil, refined	5615003	4
Phönix/Lamotte	Almond oil, refined	5615003	5
lamotte	Almond oil, refined	5615003	1

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Supplier	Substance	Batch	Spectra
Henry Lamotte Oils GmbH...	Almond oil, refined	5615003	1
Lamotte	Almond oil, refined	5669601	1
Henry Lamotte Oils GmbH	Almond oil, refined	5703001	2
Henry Lamotte Olis GmbH...	Almond oil, refined	5703001	6
Caelo	Almond oil, refined	5703001	2
Lamotte/Phoenix	Almond oil, refined	5703001	1
Henry Lamotte / Noweda	Almond oil, refined	5703001	1
Lamotte über Phoenix	Almond oil, refined	5703001	1
Lamotte/Gehe	Almond oil, refined	5703101	2
Lamotte	Almond oil, refined	5703101	1
Henry Lamotte	Almond oil, refined	5703101	2
Euro OTC	Almond oil, refined	5703101	1
Lamotte / Gehe	Almond oil, refined	5703101	1
Henry Lamotte	Almond oil, refined	5748401	1
Noweda/Henry Lamotte	Almond oil, refined	5748501	1
Henry Lamotte Oils GmbH...	Almond oil, refined	5748601	3
Stumpf/Henry Lamotte	Almond oil, refined	5748601	2
Lamotte / Noweda	Almond oil, refined	5748601	2
Henry Lamotte	Almond oil, refined	5748601	3
Lamotte über Phoenix	Almond oil, refined	5748601	3
Lamotte / Alliance Heal...	Almond oil, refined	5748601	1
Lamotte	Almond oil, refined	5748601	1
Lamotte/Phoenix	Almond oil, refined	5748601	2
Noweda	Almond oil, refined	5748601	2
lamotte/Phönix	Almond oil, refined	5748601	1
Lamotte/ Phoenix	Almond oil, refined	5748601	1
Stumpf/Henry Lamotte	Almond oil, refined	5919600001	2
Henry Lamotte Oils/Sana...	Almond oil, refined	5919600001	1
Henry Lamotte Olis GmbH...	Almond oil, refined	5919600001	1
Lamotte	Almond oil, refined	5919600001	1
Henry Lamotte	Almond oil, refined	5919600001	6
Noweda/Lamotte	Almond oil, refined	5919600001	1
Henry Lamotte Oils GmbH	Almond oil, refined	5919600001	1
Lamotte/Anzag	Almond oil, refined	8000712001	4
Lamotte	Almond oil, refined	8000712001	1
Henry Lamotte	Almond oil, refined	8000712001	3
Noweda/Lamotte	Almond oil, refined	8000712001	3
lamotte/noweda	Almond oil, refined	8000712001	2
Lamotte über Phoenix	Almond oil, refined	8000712001	2
Caelo	Almond oil, refined	8000712001	1
Henry Lamotte Oils / No...	Almond oil, refined	8000712001	1
Henry Lamotte Oils GmbH	Almond oil, refined	8000712001	1
Henry Lamotte / Kehr	Almond oil, refined	8000712001	2
Henry Lamotte/Kehr	Almond oil, refined	8000725001	1
Lamotte	Almond oil, refined	8000725001	1
Henry Lamotte/Noweda	Almond oil, refined	8000725001	1
Henry Lamotte Olis GmbH...	Almond oil, refined	8000915001	2
Henry Lamotte Oils	Almond oil, refined	8000725001	1
Henry Lamotte	Almond oil, refined	8000915001	2
Lamotte	Almond oil, refined	8000915002	1
AHD/ Henry Lamotte	Almond oil, refined	8000915002	1
Caelo	Almond oil, refined		2
Biopräp / GEHE	Almond oil, refined	E1403027	1
Bombastus	Almond oil, refined	267099	2
Biopräp / GEHE	Almond oil, refined	E1410088	1
Bombastus	Almond oil, refined	269484	1
Bombastus	Almond oil, refined	270829	1
Bombastus	Almond oil, refined	270830	1
Bombastus	Almond oil, refined	273578	3
anzag, 05.11.2012	Almond oil, refined	273578	1

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Supplier	Substance	Batch	Spectra
Phönix 15.03.2013	Almond oil, refined	273579	1
Bombastus	Almond oil, refined	274564	1
Taoasis	Almond oil, refined	102235-111893	1
HenryLamotte/Gehe	Almond oil, refined	130145	3
Henry Lamotte Gmbh, Mer...	Almond oil, refined	130145	1
Fiebig 21.02.13 ek: 2,16EUR	Almond oil, refined	130145	1
Henry Lamotte Oils GmbH	Almond oil, refined	130145	2
Phönix 16.03.2013	Almond oil, refined	130145	2
Caelo	Almond oil, refined	130145	4
Henry Lamotte	Almond oil, refined	130145	2
Lamotte/Noweda	Almond oil, refined	130145	3
H.Lamotte/Noweda	Almond oil, refined	130145	2
Henry Lamotte Oils/Sana...	Almond oil, refined	130145	1
Lamotte	Almond oil, refined	130145	7
Lamotte/Anzag	Almond oil, refined	130145	1
Henry Lamotte Oils GmbH...	Almond oil, refined	130145	1
AHD	Almond oil, refined	130145	1
Erika apotheke	Almond oil, refined	130415	1
Noweda / Henry Lamotte	Almond oil, refined	130145	1
Eigenherstellung	Almond oil, refined	21112HML01	1
Caelo	Almond oil, refined	21112PML01	1
Caelo	Almond oil, refined	3236406	1
Taoasis	Almond oil, refined	3548810	1
Primavera	Almond oil, refined	3808131	2
Caelo	Almond oil, refined	4061202	1
Primavera	Almond oil, refined	4811131	1
Eigenherstellung	Almond oil, refined	40613PML01	1
Eigenherstellung	Almond oil, refined	40613PML02	1
Eigenherstellung	Almond oil, refined	40613HML01	1
Eigenherstellung	Almond oil, refined	50612HML01	1
Caelo	Almond oil, refined	514Q1950	1
Caelo	Almond oil, refined	5111208	1
Caelo	Almond oil, refined	6081202	1
Eigenherstellung	Almond oil, refined	60913HJK01	1
Caelo	Almond oil, refined	7091206	1
Eigenherstellung	Almond oil, refined	80213HJK02	1
Caelo	Almond oil, refined	1113E-01950	1
Caelo	Almond oil, refined	914E1950	1
Caelo	Almond oil, refined	11227407	1
Caelo	Almond oil, refined	11227406	1
Caelo	Almond oil, refined	1131303	1
Caelo	Almond oil, refined	11314201	1
Caelo	Almond oil, refined	11314206	2
Noweda	Almond oil, refined	11314209	1
Caelo	Almond oil, refined	11314210	1
Caelo	Almond oil, refined	11314208	1
Caelo	Almond oil, refined	11314209	3
Taoasis	Almond oil, refined	118979-108698	1
Phönix	Almond oil, refined	12041801	2
Caelo	Almond oil, refined	12041801	10
Taoasis	Almond oil, refined	119249-109910	1
Caelo	Almond oil, refined	12041802	1
Noweda	Almond oil, refined	12041803	2
Caelo	Almond oil, refined	12041803	2
Euro OTC	Almond oil, refined	1207014-01	3
Henry Lamotte	Almond oil, refined	12061302	1
Caelo	Almond oil, refined	12080801	3
Noweda	Almond oil, refined	12080802	1
Caelo	Almond oil, refined	12080802	3
Caelo	Almond oil, refined	12080803	7

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Supplier	Substance	Batch	Spectra
Noweda	Almond oil, refined	12080803	2
Caelo	Almond oil, refined	12080806	6
Noweda	Almond oil, refined	12080806	1
Caelo	Almond oil, refined	12153501	5
Phönix Gotha	Almond oil, refined	12153501	1
Caelo	Almond oil, refined	12153502	3
Caelo	Almond oil, refined	12153505	5
Caelo	Almond oil, refined	12153506	4
phönix	Almond oil, refined	12153505	1
Caelo	Almond oil, refined	12357101	17
Noweda	Almond oil, refined	12357101	2
Anzag 09.02.2013	Almond oil, refined	12357101	1
Caelo	Almond oil, refined	12357102	6
Caelo	Almond oil, refined	12357103	7
Caelo	Almond oil, refined	12357110	1
Caelo	Almond oil, refined	12357111	6
Caelo	Almond oil, refined	12367101	1
Fagron	Almond oil, refined	12A18-N09	1
Fagron	Almond oil, refined	12J26-N05	1
Euro OTC	Almond oil, refined	1301001-02	2
J.H.Müller/direkt/01.08....	Almond oil, refined	130327	2
J.H.Müller/direkt/17.05....	Almond oil, refined	130103	1
Caelo	Almond oil, refined	13091308	1
Caelo	Almond oil, refined	13101203	1
Caelo	Almond oil, refined	1312Q-01950	1
Caesar & Loretz GmbH	Almond oil, refined	13178002	1
Caelo	Almond oil, refined	13178003	17
Phönix , 03.09.13	Almond oil, refined	13178003	1
Noweda	Almond oil, refined	13178003	1
Gehe	Almond oil, refined	13178004	1
Caelo	Almond oil, refined	13178009	2
Caelo	Almond oil, refined	13178011	11
Caelo	Almond oil, refined	132363403	1
Caelo	Almond oil, refined	13236401	16
Gehe	Almond oil, refined	13236403	1
Caelo	Almond oil, refined	13236403	4
Caelo	Almond oil, refined	13236406	9
Sanacorp	Almond oil, refined	13236406	1
Caesar & Loretz GmbH	Almond oil, refined	13236404	1
Noweda	Almond oil, refined	13236411	2
Caelo	Almond oil, refined	1326403	1
Krieger	Almond oil, refined	13350006	1
Sanacorp	Almond oil, refined	13350007	1
Caesar & Loretz GmbH	Almond oil, refined	13350007	1
Fagron	Almond oil, refined	13C25-N20	1
Caelo	Almond oil, refined	13H08-N11	1
Eigenherstellung	Almond oil, refined	140113HML01	1
Caelo	Almond oil, refined	140113PML01	1
Caelo	Almond oil, refined	1404206	1
Caelo	Almond oil, refined	14139301	1
Primavera	Almond oil, refined	15510141	1
Primavera	Almond oil, refined	1551041	2
Caelo	Almond oil, refined	1601311950	1
Caelo	Almond oil, refined	1602211950	1
Eigenherstellung	Almond oil, refined	160414HML01	1
Caelo	Almond oil, refined	17121303	1
Caelo	Almond oil, refined	17021405	1
Caelo	Almond oil, refined	20081301	1
Caelo	Almond oil, refined	2002311950	1
Caelo	Almond oil, refined	2013U01950	1

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Supplier	Substance	Batch	Spectra
Eigenherstellung	Almond oil, refined	210313HJK01	2
Caelo	Almond oil, refined	21011304	1
Caelo	Almond oil, refined	21021303	1
Caelo	Almond oil, refined	22071303	1
Caelo	Almond oil, refined	20150612-2	1
Caelo	Almond oil, refined	22081205	1
Caelo	Almond oil, refined	22111301	1
Eigenherstellung	Almond oil, refined	240214HJK01	1
Bombastus	Almond oil, refined	276542	3
Caelo	Almond oil, refined	2713U1950	1
Caelo	Almond oil, refined	2405211950	1
Gehe 06.05.2013	Almond oil, refined	276611	1
Caelo	Almond oil, refined	25041303	1
Bombastus	Almond oil, refined	277912	2
Bombastus	Almond oil, refined	279230	1
Bombastus	Almond oil, refined	281765	1
Bombastus	Almond oil, refined	282093	1
Caelo	Almond oil, refined	31121205	1
Caelo	Almond oil, refined	4313E1950	1
H. Lamotte	Almond oil, refined	5120901	1
Lamotte/Anzag 30.06.2012	Almond oil, refined	5162801	2
Lamotte/Anzag 12.06.2012	Almond oil, refined	5177001	1
Henry Lamotte	Almond oil, refined	5177001	3
H. Lamotte	Almond oil, refined	5177001	3
Noweda	Almond oil, refined	5177001	4
Henry Lamotte/Anzag	Almond oil, refined	5177001	1
henry Lamotte	Almond oil, refined	5177001	1
Lamotte/Krieger	Almond oil, refined	5177001	1
ANZAG	Almond oil, refined	5214206	1
Lamotte/Sanacorp	Almond oil, refined	5214206	1
Caelo	Almond oil, refined	5214206	3
Lamotte/gehe	Almond oil, refined	5214206	1
Phönix/Lamotte	Almond oil, refined	5214206	3
Lamotte Phönix	Almond oil, refined	5214206	1
Noweda / Henry Lamotte	Almond oil, refined	5214206	3
Lamotte	Almond oil, refined	5214206	3
Sanacorp	Almond oil, refined	5214206	2
Henry Lamotte Oils GmbH	Almond oil, refined	5214206	1
H.Lamotte/Noweda	Almond oil, refined	5214206	1
Henry Lamotte	Almond oil, refined	5214206	1
Anzag	Almond oil, refined	5214206	1
Kehr / Lamotte	Almond oil, refined	5214206	1
Noweda	Almond oil, refined	5269301	4
Sanacorp	Almond oil, refined	5269301	2
Henry Lamotte Oils GmbH	Almond oil, refined	5269301	2
Klenk	Almond oil, refined	5269301	2
H.Lamotte/Noweda	Almond oil, refined	5269301	2
Phönix/Lamotte	Almond oil, refined	5269301	3
Henry Lamotte GmbH	Almond oil, refined	5269301	1
HenryLamotte/Phoenix	Almond oil, refined	5269301	2
Lamotte/Krieger	Almond oil, refined	5269301	2
Lamotte	Almond oil, refined	5269301	3
Phoenix (Henry Lamotte ...	Almond oil, refined	5269301	1
Lamotte/gehe	Almond oil, refined	5274206	1
Lamotte/Phoenix	Almond oil, refined	5415901	2
Phoenix	Almond oil, refined	5269301	1
Henry Lamotte	Almond oil, refined	5369301	1
Phoenix/Lamotte	Almond oil, refined	5415901	1
Stumpf/Henry Lamotte	Almond oil, refined	5415901	2
Lamotte/ Noweda	Almond oil, refined	5415901	1

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Supplier	Substance	Batch	Spectra
LAMOTTE/NOWEDA	Almond oil, refined	5415901	4
Sanacorp	Almond oil, refined	5415901	2
Henry Lamotte	Almond oil, refined	5415901	3
lamotte/anzag	Almond oil, refined	5415901	3
Lamotte/Ebert	Almond oil, refined	5415901	1
Henry Lamotte Oils Gmbh	Almond oil, refined	5415901	1
H.Lamotte/Noweda	Almond oil, refined	5415901	1
Phönix	Almond oil, refined	543801	1
Henry Lamotte	Almond oil, refined	5438301	4
Henry Lamotte	Almond oil, refined	543802	1
Großhandel	Almond oil, refined	5438301	5
Henry Lamotte/ 11.05.13. . .	Almond oil, refined	5438301	1
Phönix/Lamotte	Almond oil, refined	5438301	10
Noweda / Henry Lamotte	Almond oil, refined	5438301	3
Henry Lamotte OilsGmbH	Almond oil, refined	5438301	1
Caelo	Almond oil, refined	5438301	4
Lamotte	Almond oil, refined	5438301	6
Henry Lamotte/Phönix	Almond oil, refined	5438301	1
Phönix	Almond oil, refined	5438301	1
Lamotte/Noweda	Almond oil, refined	5438301	1
Fischar	Almond oil, refined	5438301	2
H.Lamotte/Noweda	Almond oil, refined	5438301	2
Anzag	Almond oil, refined	5438301	2
lamotte	Almond oil, refined	5438301	1
Lamotte/ Noweda	Almond oil, refined	5438301	1
Phönix, 17.06.2013	Almond oil, refined	5438301	1
Henry Lamotte Oils GmbH. . .	Almond oil, refined	5438301	1
Großhandel	Almond oil, refined	5438302	1
Stumpf/Henry Lamotte	Almond oil, refined	5438302	4
Lamotte/GEHE	Almond oil, refined	5438302	3
Henry Lam. / Phönix	Almond oil, refined	5438302	1
Henry Lamotte	Almond oil, refined	5438302	4
Noweda/Lamotte	Almond oil, refined	5438302	3
Caelo	Almond oil, refined	5438302	3
Sanacorp	Almond oil, refined	5438302	1
AHC03.08.13 EK2,36 100ml	Almond oil, refined	5438302	1
Henry Lamotte Oils, Gehe	Almond oil, refined	5438302	1
H.Lamotte/Noweda	Almond oil, refined	5438302	2
HenryLamotteOilsGmbH/Ph. . .	Almond oil, refined	5438302	2
H.Lamotte/Anzag	Almond oil, refined	5438302	1
Lamotte	Almond oil, refined	5438302	4
Henry Lamotte Oils GmbH	Almond oil, refined	5438302	1
noweda/Ichtyol	Almond oil, refined	5438302	2
Lamotte/Sanacorp	Almond oil, refined	5438302	1
Lamotte/ Phönix	Almond oil, refined	5438302	1
Taoasis	Almond oil, refined	5452701-111406	1
H.Lamotte / Anzag	Almond oil, refined	5438302	1
Kruger/Lamotte/06.01.14	Almond oil, refined	5438302	1
Taoasis	Almond oil, refined	5452701-111421	1
Henry Lamotte Oils GmbH	Almond oil, refined	5493001	1
Henry Lamotte Oils GmBH. . .	Almond oil, refined	5438302	1
Stumpf/Henry Lamotte	Almond oil, refined	5493001	4
Henry Lamotte	Almond oil, refined	5493001	3
Lamotte / Alliance Heal. . .	Almond oil, refined	5438302	1
Henry Lamotte Oils GmbH. . .	Almond oil, refined	5493001	1
Henry Lamotte Oils GmbH. . .	Almond oil, refined	5493001	1
Taoasis	Almond oil, refined	5511701-1113571	1
Caelo	Almond oil, refined	5615001	3
H.Lamotte/Noweda	Almond oil, refined	5615001	2
lamotte/Noweda	Almond oil, refined	5615001	1

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Supplier	Substance	Batch	Spectra
Phönix	Almond oil, refined	5669601	1
Henry Lamotte	Almond oil, refined	5615003	1
Spinnrad GmbH	Almond oil, refined	913301224	1
Spinnrad GmbH	Almond oil, refined	713301223	1
Lamotte/gehe	Almond oil, refined	74760	2
xxx	Almond oil, refined		1
Lamotte / Gehe	Evening primrose oil, refined	124363	4
Lamotte / Noweda	Evening primrose oil, refined	145581	3
Lamotte//AHD	Evening primrose oil, refined	145581	2
Lamotte / Gehe	Evening primrose oil, refined	145802	9
Lamotte / Gehe	Evening primrose oil, refined	150827	4
Phönix	Evening primrose oil, refined	150827	1
taoasis/Noweda	Evening primrose oil, refined	37282-115267	1
Caelo	Evening primrose oil, refined	5011508	1
Caelo	Evening primrose oil, refined	7011502	1
Caelo	Evening primrose oil, refined	5061505	1
Taoasis	Evening primrose oil, refined	120161-93968	1
Lamotte/AHD	Evening primrose oil, refined	10000001044	1
Caelo	Evening primrose oil, refined	10101404	1
Caelo	Evening primrose oil, refined	12031604	1
Euro OTC	Evening primrose oil, refined	1210012-01	12
Euro OTC	Evening primrose oil, refined	1210012-02	9
Caelo	Evening primrose oil, refined	1210012-02	1
Euro OTC	Evening primrose oil, refined	1304018-01	9
Euro OTC	Evening primrose oil, refined	1304018-02	9
Großhandel	Evening primrose oil, refined	1304018-02	1
Caelo	Evening primrose oil, refined	13121812	8
Caelo	Evening primrose oil, refined	13121816	12
Caelo	Evening primrose oil, refined	14002501	1
Caelo	Evening primrose oil, refined	14002503	7
Euro OTC	Evening primrose oil, refined	1401033-01	7
Phoenix	Evening primrose oil, refined	1401033-01	1
Euro OTC	Evening primrose oil, refined	1401033-02	8
Caelo	Evening primrose oil, refined	14010901	1
Noweda	Evening primrose oil, refined	14010904	1
Phoenix 04.12.14	Evening primrose oil, refined	14010905	1
Caelo	Evening primrose oil, refined	14010903	1
Gehe	Evening primrose oil, refined	14010904	1
Caelo	Evening primrose oil, refined	14010908	10
Gehe	Evening primrose oil, refined	14010908	1
Caelo	Evening primrose oil, refined	14010910	7
Caelo	Evening primrose oil, refined	14010912	1
Caelo	Evening primrose oil, refined	14010913	8
Caesar & Loretz GmbH	Evening primrose oil, refined	14010910	1
Caelo	Evening primrose oil, refined	14010915	7
phönix	Evening primrose oil, refined	14010915	1
Caelo	Evening primrose oil, refined	14010914	2
Caelo	Evening primrose oil, refined	14010918	4
Caelo	Evening primrose oil, refined	14010920	1
Caelo	Evening primrose oil, refined	14010980	1
J.H. Müller	Evening primrose oil, refined	140419	1
Caelo	Evening primrose oil, refined	1401908	1
Caelo	Evening primrose oil, refined	1407002-01	1
Caelo	Evening primrose oil, refined	1401904	1
Euro OTC	Evening primrose oil, refined	1407002-01	8
Euro OTC	Evening primrose oil, refined	140700201	2
Euro OTC	Evening primrose oil, refined	140700202	2
Euro OTC	Evening primrose oil, refined	1407002-02	12
Gehe 5.03.15	Evening primrose oil, refined	1407002-02	1
Spirig /Noweda	Evening primrose oil, refined	1407002-01	1

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Supplier	Substance	Batch	Spectra
Caelo	Evening primrose oil, refined	1407002-02	1
Caelo	Evening primrose oil, refined	14258601	8
Caelo	Evening primrose oil, refined	14258603	5
Phoenix	Evening primrose oil, refined	14258604	1
Caelo	Evening primrose oil, refined	14258604	3
Caelo	Evening primrose oil, refined	14258606	8
Caelo	Evening primrose oil, refined	14258607	1
Caelo	Evening primrose oil, refined	14258608	9
Fagron	Evening primrose oil, refined	14258608	1
Caelo	Evening primrose oil, refined	14258610	13
Caelo	Evening primrose oil, refined	14258611	3
Caesar & Loretz GmbH	Evening primrose oil, refined	14258611	1
Caelo	Evening primrose oil, refined	14258612	2
Caelo	Evening primrose oil, refined	14258616	11
Caelo	Evening primrose oil, refined	14258617	8
Phoenix	Evening primrose oil, refined	14258617	2
Euro OTC	Evening primrose oil, refined	14C07-B01-291800	1
Fagron	Evening primrose oil, refined	14C07-801-291800	1
Caelo	Evening primrose oil, refined	1428616	1
Fagron	Evening primrose oil, refined	14C07-B01-291800	1
Fagron	Evening primrose oil, refined	14H18-B04-267707	1
Fagron	Evening primrose oil, refined	14H18-B04-297707	1
Caelo	Evening primrose oil, refined	150081403	1
Ph.Eur.8.2	Evening primrose oil, refined	14H18B04297708	1
Euro OTC	Evening primrose oil, refined	1503031-01	9
Euro OTC	Evening primrose oil, refined	150303101	1
Euro OTC	Evening primrose oil, refined	1506001-01	7
EuRho	Evening primrose oil, refined	1506001-01	1
Rondell Apotheke	Evening primrose oil, refined	1506001-01	1
Caelo	Evening primrose oil, refined	15081401	3
Caelo	Evening primrose oil, refined	15081403	6
Caelo	Evening primrose oil, refined	15081402	2
Caelo	Evening primrose oil, refined	15081404	7
Caelo	Evening primrose oil, refined	15081405	14
Caelo	Evening primrose oil, refined	15081407	6
Euro OTC	Evening primrose oil, refined	1509005-01	4
EuRho	Evening primrose oil, refined	1509005-01	2
Euro OTC	Evening primrose oil, refined	1512005-01	6
Euro/Sanacorp	Evening primrose oil, refined	1512005-01	1
Euro OTC	Evening primrose oil, refined	1512005-02	6
Euro/Phoenix	Evening primrose oil, refined	1512005-02	2
Caelo	Evening primrose oil, refined	15171101	2
Caelo	Evening primrose oil, refined	15121405	1
Caelo	Evening primrose oil, refined	15171102	15
Caelo	Evening primrose oil, refined	15141102	1
Caelo	Evening primrose oil, refined	15171103	3
Caelo	Evening primrose oil, refined	15171104	10
Caesar & Loretz GmbH	Evening primrose oil, refined	15171104	1
Caelo	Evening primrose oil, refined	15171105	3
Caelo	Evening primrose oil, refined	15171109	6
Caesar & Loretz GmbH	Evening primrose oil, refined	15171109	1
Caelo	Evening primrose oil, refined	15171110	14
Noweda	Evening primrose oil, refined	15171109	1
Caelo	Evening primrose oil, refined	15171111	6
Caelo	Evening primrose oil, refined	15417801	13
Caelo	Evening primrose oil, refined	15417802	17
Wolf-Apotheke	Evening primrose oil, refined	15417802	2
Caelo	Evening primrose oil, refined	154178020	1
Phoenix	Evening primrose oil, refined	15417803	1
Caelo	Evening primrose oil, refined	15417803	4

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Supplier	Substance	Batch	Spectra
Caelo	Evening primrose oil, refined	15417805	2
Euro OTC	Evening primrose oil, refined	1603048-01	3
Caelo	Evening primrose oil, refined	15417809	1
Caelo	Evening primrose oil, refined	15417806	1
Euroo/Gehe	Evening primrose oil, refined	1603048-01	1
Caelo	Evening primrose oil, refined	30031501	1
Euro OTC	Evening primrose oil, refined	1813M-03075	1
Taoasis	Evening primrose oil, refined	3788-116147	1
Taoasis	Evening primrose oil, refined	3843-121697	2
Caelo	Evening primrose oil, refined	458528	1
Audor Pharma	Evening primrose oil, refined	392-133N	1
Audor Pharma	Evening primrose oil, refined	AP294-118N	7
Audor Pharma	Evening primrose oil, refined	AP392-133N	3
Audor Pharma	Evening primrose oil, refined	AP562-124N	6
Audor Pharma	Evening primrose oil, refined	AP273-116N	4
Audor Pharma	Evening primrose oil, refined	AP396-120N	4
Allianz Healthcare 01.0...	Evening primrose oil, refined	AP562-124N	2
Audor Pharma	Evening primrose oil, refined	AP-788-128N	1
Audor Pharma	Evening primrose oil, refined	AP788-128N	4
Bergland/Anzag	Evening primrose oil, refined	H500690	1
Bergland/Phönix	Evening primrose oil, refined	H302605	1
Bergland/Phönix	Evening primrose oil, refined	K501908	1
Caelo	Evening primrose oil, refined	122966	3
Bergland	Evening primrose oil, refined	K6013776	1
Klenk	Evening primrose oil, refined	122966	4
Lamotte	Evening primrose oil, refined	123121	1
Lamotte / Gehe	Evening primrose oil, refined	123121	3
Henry Lamotte	Evening primrose oil, refined	123121	1
Lamotte / Gehe	Evening primrose oil, refined	123386	7
Lamotte	Evening primrose oil, refined	145553	1
Anzag 30.05.2012	Evening primrose oil, refined	144906	1
Lamotte / Gehe	Evening primrose oil, refined	145553	5
Lamotte / Gehe	Evening primrose oil, refined	145675	4
Anzag/Henry Lamotte	Evening primrose oil, refined	145675	1
Lamotte / Gehe	Evening primrose oil, refined	145691	14
Stumpf/Henry Lamotte	Evening primrose oil, refined	145691	1
Caelo	Evening primrose oil, refined	2011409	1
Caelo	Evening primrose oil, refined	4061305	1
Euro OTC	Evening primrose oil, refined	80616-11	1
Euro OTC	Evening primrose oil, refined	1109004-01	1
Caelo	Evening primrose oil, refined	11019201	1
Gehe	Evening primrose oil, refined	1109004-02	1
Caesar & Loretz GmbH 40...	Evening primrose oil, refined	11150007	1
Caelo	Evening primrose oil, refined	12032901	1
Caelo	Evening primrose oil, refined	12032906	2
Gehe	Evening primrose oil, refined	12032908	1
Caelo	Evening primrose oil, refined	12032908	2
Caelo	Evening primrose oil, refined	12032912	2
Caelo	Evening primrose oil, refined	12032913	2
Caesar & Loretz GmbH, 4...	Evening primrose oil, refined	12032913	1
Noweda	Evening primrose oil, refined	12032910	1
Euro OTC	Evening primrose oil, refined	1205023-01	5
Anzag ek:13.04EUR 08.08.12	Evening primrose oil, refined	1205023-01	2
Phönix 17.08.2012	Evening primrose oil, refined	1205023-01	2
Noweda	Evening primrose oil, refined	1205023-01	5
Caelo	Evening primrose oil, refined	120502302	1
Fagron	Evening primrose oil, refined	1205023-02	1
Caelo	Evening primrose oil, refined	1205023-02	2
Euro OTC	Evening primrose oil, refined	1205023-02	6
Gehe	Evening primrose oil, refined	1205023-02	1

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Supplier	Substance	Batch	Spectra
Anzag 30.01.13 ek:16,40EUR	Evening primrose oil, refined	1205023-02	1
Großhandel	Evening primrose oil, refined	1205023-02	1
Caelo	Evening primrose oil, refined	120543078-13	1
Euro OTC	Evening primrose oil, refined	1205023-1	1
Caelo	Evening primrose oil, refined	1210012-01	1
EuRho	Evening primrose oil, refined	1210012-02	3
Jenne	Evening primrose oil, refined	1210012-02	1
phönix	Evening primrose oil, refined	1210012-02	1
Gehe	Evening primrose oil, refined	121112906	1
Caelo	Evening primrose oil, refined	12112901	2
Fiebig 12.07.13 EK15,38...	Evening primrose oil, refined	1210012-02	1
noveda	Evening primrose oil, refined	12112901	1
ANZAG 27.12.2012	Evening primrose oil, refined	12112901	1
Caelo	Evening primrose oil, refined	12112902	2
Caelo	Evening primrose oil, refined	12112903	1
Caelo	Evening primrose oil, refined	12112905	4
Noweda	Evening primrose oil, refined	12112905	2
Klenk	Evening primrose oil, refined	12112905	1
Kehr	Evening primrose oil, refined	12112906	1
Caelo	Evening primrose oil, refined	12112906	2
Gehe	Evening primrose oil, refined	12112906	1
Euro OTC	Evening primrose oil, refined	12112906	1
Caelo	Evening primrose oil, refined	12112908	5
Caelo	Evening primrose oil, refined	12112910	1
Caesar & Loretz GmbH, 4...	Evening primrose oil, refined	12112911	1
Caelo	Evening primrose oil, refined	12112911	4
Caelo	Evening primrose oil, refined	12112912	1
Ichthyl Phönix	Evening primrose oil, refined	12112912	1
Caelo	Evening primrose oil, refined	12112914	1
Caelo	Evening primrose oil, refined	12112915	2
Hustadt Apotheke	Evening primrose oil, refined	1211905	1
Caelo	Evening primrose oil, refined	12325101	8
Fagron	Evening primrose oil, refined	12325101	2
Caesar & Loretz GmbH, 4...	Evening primrose oil, refined	12325101	1
Noweda	Evening primrose oil, refined	12325101	1
Caelo	Evening primrose oil, refined	12325103	5
Caelo	Evening primrose oil, refined	12325105	6
Caelo	Evening primrose oil, refined	12325106	15
Kehr	Evening primrose oil, refined	12325106	1
Caesar & Loretz GmbH, 4...	Evening primrose oil, refined	12325106	1
Gehe	Evening primrose oil, refined	12325106	1
Caelo	Evening primrose oil, refined	12325107	8
Caesar & Loretz GmbH	Evening primrose oil, refined	12325107	1
Caelo	Evening primrose oil, refined	12325109	5
Gehe	Evening primrose oil, refined	12325110	1
Caelo	Evening primrose oil, refined	12325110	2
Caelo	Evening primrose oil, refined	12325111	11
Sanacorp	Evening primrose oil, refined	12325111	1
Caesar & Loretz GmbH, 4...	Evening primrose oil, refined	12325113	1
Caelo	Evening primrose oil, refined	12325113	5
Gehe	Evening primrose oil, refined	12325113	1
Caelo	Evening primrose oil, refined	12325114	4
Sanacorp	Evening primrose oil, refined	12325114	1
Caelo	Evening primrose oil, refined	12325115	3
Caelo	Evening primrose oil, refined	12325116	3
Caelo	Evening primrose oil, refined	1232516	1
Caelo	Evening primrose oil, refined	1235101	1
Caelo	Evening primrose oil, refined	1235113	1
Caelo	Evening primrose oil, refined	12355115	1
Caelo	Evening primrose oil, refined	1235106	1

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Supplier	Substance	Batch	Spectra
Fagron	Evening primrose oil, refined	12J08-N04	1
Fagron	Evening primrose oil, refined	12e23-N06	1
Euro/Phönix	Evening primrose oil, refined	1304018-01	2
J.H.Müller/direkt/17.05...	Evening primrose oil, refined	130127	1
Großhandel	Evening primrose oil, refined	1304018-01	1
Euro OTC	Evening primrose oil, refined	130401801	1
Phönix 27.01.2014	Evening primrose oil, refined	1304018-01	1
Euro/ Phönix	Evening primrose oil, refined	1304018-02	1
Caelo	Evening primrose oil, refined	13121804	1
Caelo	Evening primrose oil, refined	13121806	2
Bombastus	Evening primrose oil, refined	13121806	1
Caelo	Evening primrose oil, refined	13121807	7
Noweda	Evening primrose oil, refined	13121807	1
Caelo	Evening primrose oil, refined	13121808	17
Phönix 18.11.2013	Evening primrose oil, refined	13121808	1
Sanacorp	Evening primrose oil, refined	13121809	2
Caelo	Evening primrose oil, refined	13121809	9
Caesar & Loretz	Evening primrose oil, refined	13121809	1
Caesar & Loretz GmbH	Evening primrose oil, refined	13121812	1
Sanacorp	Evening primrose oil, refined	13121814	1
Caelo	Evening primrose oil, refined	13121813	3
Caelo	Evening primrose oil, refined	13121814	3
Caerl/Phönix	Evening primrose oil, refined	13121814	1
celo/phönix	Evening primrose oil, refined	13121814	1
Cealo / Noweda	Evening primrose oil, refined	13121814	1
Caelo	Evening primrose oil, refined	13121818	3
Herbasinica	Evening primrose oil, refined	1312809	2
Caelo	Evening primrose oil, refined	1312812	1
Fagron	Evening primrose oil, refined	13E06-N09	3
Fargron	Evening primrose oil, refined	13E06-N09	1
Caelo	Evening primrose oil, refined	14002502	2
Caelo	Evening primrose oil, refined	14010904	3
müller	Evening primrose oil, refined	1401332X	1
Lamotte	Evening primrose oil, refined	145675	1
Euro OTC	Evening primrose oil, refined	1506001	1
dr.r.hahn	Evening primrose oil, refined	1509005-01	1
Caelo	Evening primrose oil, refined	160213003	1
Caelo	Evening primrose oil, refined	20140612-18	1
Caelo	Evening primrose oil, refined	3112M-03075	1
PG-Naturpharma/Sanacorp	Evening primrose oil, refined	711-098	1
weltecke/Noweda	Evening primrose oil, refined	80010212	1
Audor Pharma	Evening primrose oil, refined	869-100N	1
Audor Pharma	Evening primrose oil, refined	AP869-100/1N	1
Audor Pharma	Evening primrose oil, refined	AP191-088N	2
Audor Pharma	Evening primrose oil, refined	AP920-114N	8
Audor Pharma	Evening primrose oil, refined	AP094-115N	1
Audor Pharma	Evening primrose oil, refined	AP191-088/1N	1
Audor Pharma	Evening primrose oil, refined	AP366-108N	3
Audor Pharma	Evening primrose oil, refined	AP869-100N	1
Audor Pharma	Evening primrose oil, refined	AP676-078N	1
Phoenix	Evening primrose oil, refined	AP869100N	1
Audor Pharma	Evening primrose oil, refined	AP920-114/1N	1
Audor Pharma	Evening primrose oil, refined	Ap869-100N	1
allcura	Evening primrose oil, refined	L2641	1
Caelo	Flaxseed oil, native	15175604	1
Caelo	Flaxseed oil, native	15415906	2
Caelo	Flaxseed oil, native	263894	1
Euro OTC	Flaxseed oil, native	13058506	1
Caelo	Flaxseed oil, native	13178210	2
statfold	Flaxseed oil, native	8001-26-1	1

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Supplier	Substance	Batch	Spectra
Henry Lamotte/ Noweda	Olive oil, native	124392	1
Caelo	Olive oil, native	1081402	1
Caelo	Olive oil, native	2061503	1
Bombastus	Olive oil, native	6861571	2
Caelo	Olive oil, native	5011503	1
Fagron	Olive oil, native	129189	1
Fagron	Olive oil, native	130190	1
Fagron	Olive oil, native	133026	2
Caelo	Olive oil, native	13051402	1
Caelo	Olive oil, native	13350102	17
PHOENIX 03.03.2014	Olive oil, native	1305014-01	1
Caesar & Loretz GmbH Hi...	Olive oil, native	13350102	1
Caelo	Olive oil, native	13350103	12
Fagron	Olive oil, native	13J25-B04	1
Caelo	Olive oil, native	13350104	6
Caelo	Olive oil, native	14024407	8
Caelo	Olive oil, native	14024408	10
Caelo	Olive oil, native	14024409	6
Euro OTC	Olive oil, native	1406009-01	1
Caelo	Olive oil, native	14070802	1
Caelo	Olive oil, native	14071504	1
Caelo	Olive oil, native	14118603	15
Phoenix	Olive oil, native	14118603	1
Caelo	Olive oil, native	14118604	10
Caelo	Olive oil, native	14118606	6
Caelo	Olive oil, native	14182301	4
Phönix	Olive oil, native	14118606	1
Caelo	Olive oil, native	14182302	9
Noweda 21.02.2015	Olive oil, native	14182302	1
Caelo	Olive oil, native	14182303	11
Caelo	Olive oil, native	14182304	7
Caelo	Olive oil, native	14306903	3
Caelo	Olive oil, native	14306902	1
Caelo	Olive oil, native	14306904	7
sanacorp	Olive oil, native	14306904	1
Caesar & Loretz GmbH	Olive oil, native	14306904	1
Bombastus	Olive oil, native	14306904	1
Caelo	Olive oil, native	14306905	9
Caelo	Olive oil, native	14306915	5
Caelo	Olive oil, native	14306916	9
Caelo	Olive oil, native	14306906	3
Caelo	Olive oil, native		1
Fagron	Olive oil, native	14B12-B06	1
Fagron	Olive oil, native	14G08-B02-300074	3
Caelo	Olive oil, native	15112704	1
Caelo	Olive oil, native	15112703	1
Caelo	Olive oil, native	15112705	7
sanacorp	Olive oil, native	15112706	1
Caelo	Olive oil, native	15112706	7
Caelo	Olive oil, native	15216307	8
Caelo	Olive oil, native	15112707	3
Caelo	Olive oil, native	15216308	5
Phönix Gotha	Olive oil, native	15216308	1
Caesar & Loretz GmbH Hi...	Olive oil, native	15216309	1
Caelo	Olive oil, native	15311401	3
Caelo	Olive oil, native	15216309	4
Caelo	Olive oil, native	15311402	4
Caelo	Olive oil, native	15311403	10
Caelo	Olive oil, native	15311404	8
Caelo	Olive oil, native	15311408	4

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Supplier	Substance	Batch	Spectra
Caelo	Olive oil, native	15399702	6
Bombastus	Olive oil, native	15399702	1
Caelo	Olive oil, native	15399703	7
Noweda	Olive oil, native	15399702	1
Caelo	Olive oil, native	15399704	6
Phoenix	Olive oil, native	16035310	1
Caelo	Olive oil, native	16035308	2
Caelo	Olive oil, native	15399706	1
Phoenix	Olive oil, native	16035311	1
Caelo	Olive oil, native	16035310	3
PHÖNIX	Olive oil, native	16327402	1
Caelo	Olive oil, native	16035311	4
Caelo	Olive oil, native	20061502	1
Caelo	Olive oil, native	24031502	1
Bombastus	Olive oil, native	282963	7
Caelo	Olive oil, native	24081507	1
Bombastus	Olive oil, native	279608	5
gehe	Olive oil, native	282963	2
gehe	Olive oil, native	284144	2
gehe	Olive oil, native	285942	3
Bombastus	Olive oil, native	284144	7
Bombastus	Olive oil, native	285942	9
Bombastus	Olive oil, native	286533	7
Brücken-Apotheke	Olive oil, native	288752	2
Gehe	Olive oil, native	287259	1
Bombastus	Olive oil, native	288752	3
Caelo	Olive oil, native	288752	2
Caelo	Olive oil, native	290924	1
Bombastus	Olive oil, native	291374	3
Bombastus	Olive oil, native	290924	9
Caelo	Olive oil, native	2915A-02000	1
Bombastus	Olive oil, native	292369	11
Bombastus	Olive oil, native	295282	5
Caelo	Olive oil, native	294034	1
Bombastus	Olive oil, native	294034	5
Bombastus	Olive oil, native	297227	3
Bombastus	Olive oil, native	295283	7
Bombastus	Olive oil, native	296259	1
Bombastus	Olive oil, native	296260	7
Bombastus	Olive oil, native	298008	4
Bombastus	Olive oil, native	300220	5
Bombastus	Olive oil, native	301100	7
Bombastus	Olive oil, native	302523	5
Bombastus	Olive oil, native	304112	1
Bombastus	Olive oil, native	305003	1
Bombastus	Olive oil, native	3011000	1
Caelo	Olive oil, native	3916I-02000	1
Raben-Apotheke Mildenau	Olive oil, native	5623601	1
Henry Lamotte	Olive oil, native	5671601	1
Hedinger	Olive oil, native	5623601	1
Lamotte / Alliance Heal...	Olive oil, native	5671601	1
Bombastus	Olive oil, native	5671901	3
Lamotte/Anzag	Olive oil, native	5813601	1
Noweda/Lamotte	Olive oil, native	5813601	1
Raben-Apotheke Mildenau	Olive oil, native	5891202	3
Caelo	Olive oil, native	5891202	1
Henry Lamotte/Noweda	Olive oil, native	8000821001	1
Caelo	Olive oil, native	114Q-02000	1
Bombastus	Olive oil, native	273871	4
Lamotte	Olive oil, native	123773	2

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Supplier	Substance	Batch	Spectra
Henry Lamotte	Olive oil, native	8001560001	1
Henry Lamotte / Noweda	Olive oil, native	123773	1
Noweda	Olive oil, native	272270	2
Henry Lamotte/Anzag	Olive oil, native	123773	1
phönix	Olive oil, native		1
Bombastus	Olive oil, native		1
Bombastus	Olive oil, native	274236	10
Caelo	Olive oil, native	3071302	1
Caelo	Olive oil, native	11376905	3
Caelo	Olive oil, native	12077701	17
Caelo	Olive oil, native	11376906	4
Caelo	Olive oil, native	12077702	4
Caelo	Olive oil, native	12141306	11
Caelo	Olive oil, native	12141305	3
fargon	Olive oil, native	1212022-01	2
Caelo	Olive oil, native	12274104	7
Caelo	Olive oil, native	12141309	6
Caelo	Olive oil, native	12274105	1
Caelo	Olive oil, native	12274106	12
Bombastus	Olive oil, native	12274106	1
Alliance Healthcare	Olive oil, native	12274108	1
Euro OTC	Olive oil, native	12274109	3
Fagron	Olive oil, native		1
Caelo	Olive oil, native	13010904	24
celo/Jenne	Olive oil, native	13010904	1
phönix	Olive oil, native	13010904	1
Caelo	Olive oil, native	13010906	11
Gehe 13.06.2013	Olive oil, native	13010906	2
Caelo	Olive oil, native	130109062x	1
Caelo	Olive oil, native	13010911	17
Caelo	Olive oil, native	13010907	1
EuRho	Olive oil, native	13010911	1
Gehe	Olive oil, native	13010911	1
Caelo	Olive oil, native	13147001	8
Caelo	Olive oil, native	13147002	9
Caelo	Olive oil, native	13147004	17
sanacorp	Olive oil, native	13147004	1
Caelo	Olive oil, native	13224701	4
Gehe 04.11.2013	Olive oil, native	13224701	1
Caelo	Olive oil, native	13224702	4
Caelo	Olive oil, native	13224703	18
Caelo	Olive oil, native	13224704	15
Caelo	Olive oil, native	13350101	3
Noweda	Olive oil, native	13350102	1
Fagron	Olive oil, native	13C08-N06	8
Caelo	Olive oil, native	13350105	3
Sanacorp	Olive oil, native	13C08-N06	1
Fagron	Olive oil, native	13G18-B08	1
Caelo	Olive oil, native	14024406	2
Fagron	Olive oil, native	13G18-B08-286424	3
Caelo	Olive oil, native	25021404	1
Caelo	Olive oil, native	16121306	1
Bombastus	Olive oil, native	275757	2
Phönix	Olive oil, native	20032	1
Gehe	Olive oil, native	277050	2
Caelo	Olive oil, native	16011404	1
Phönix Gotha	Olive oil, native	277049	1
Noweda	Olive oil, native	277050	2
Bombastus	Olive oil, native	277050	6
Bombastus	Olive oil, native	278583	9

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Supplier	Substance	Batch	Spectra
Bombastus	Olive oil, native	279609	6
Bombastus	Olive oil, native	281898	5
Bombastus	Olive oil, native	281209	5
Caelo	Olive oil, native	28121202	1
Lamotte/ Anzag	Olive oil, native	5271504	1
Caelo	Olive oil, native	31081206	1
Bombastus	Olive oil, native	289095	3
Gehe	Olive oil, native	282963	2
H. Lamotte	Olive oil, native	5271504	1
Caelo	Olive oil, native	30071305	1
Lamotte Phönix	Olive oil, native	5271504	1
Caelo	Olive oil, native	5271504	2
lamotte/Gehe	Olive oil, native	5271504	1
Lamotte	Olive oil, native	5272401	3
Noweda/Anzag	Olive oil, native	5272401	1
Henry Lamotte, Noweda	Olive oil, native	5372701	1
Henry Lamotte	Olive oil, native	5272401	2
Lamotte	Olive oil, native	5464901	2
Henry Lamotte	Olive oil, native	5464901	1
Lamotte / Gehe	Olive oil, native	5470202	1
Gehe	Olive oil, native	5470202	1
Lamotte/ Anzag	Olive oil, native	5470202	2
Lamotte	Olive oil, native	5470202	3
Phoenix	Olive oil, native	5470202	1
H.Lamotte/Noweda	Olive oil, native	5470202	1
Caelo	Olive oil, native	90417099	1
Lamotte/AHD	Evening primrose oil, refined	124363	2
Euro OTC	Evening primrose oil, refined	140103302	1
Hedinger	Evening primrose oil, refined	14010915	5
Caelo	Evening primrose oil, refined	14010917	1
Caelo	Evening primrose oil, refined	14258615	1
Euro OTC	Evening primrose oil, refined	13040-18-01	1
Caelo	Evening primrose oil, refined	14010905	1
Caelo	Almond oil, refined	15127303	1
Caelo	Almond oil, refined	16071004	2
Caelo	Almond oil, refined	3714U-01950	1
Henry Lamotte Oils / No...	Almond oil, refined	8000915001	1
Henry Lamotte Oils GmbH...	Almond oil, refined	1714U-01950	1
Henry LAmotte Oils GmbH	Almond oil, refined	8001497001	6
Henry Lamotte / Noweda	Almond oil, refined	8000915002	1
Noweda	Almond oil, refined	11078806	1
HENRY LAMOTTE OILS GmbH	Almond oil, refined	8001497001	1
Caelo	Almond oil, refined	13236404	3
Lamotte/Krieger	Almond oil, refined	5081301	1
Henry Lamotte/N/18.06.1...	Almond oil, refined	5438301	1
Lamotte/N/31.05.13/PZN:...	Almond oil, refined	5214206	1
Noweda	Peanut oil, refined	11B16-N02	2
Caelo	Peanut oil, refined	12203806	3
Henry Lamotte GmbH/Hold...	Peanut oil, refined	5231601	1
Caelo	Avocado oil, refined	12064812	2
Caelo	Borage oil, refined, stabili...	16266007	1
Bergland	Borage oil, refined, stabili...	H300590	2
Lamotte/Noweda	Codliver oil (type A)	8000601001	3
Lamotte/ Noweda	Codliver oil (type A)	8000918001	2
Caelo	Codliver oil (type A)	8001176004	2
Henry Lamotte GmbH/Hold...	Codliver oil (type A)	5228001	2
Anzag	Codliver oil (type A)	5228001	2
Caelo	Jojoba oil, native	14052206	1
Bombastus	Jojoba oil, native	267834	1
Caelo	Jojoba oil, native	2614A-01986	1

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Supplier	Substance	Batch	Spectra
Caelo	Jojoba oil, native	14284207	1
Caelo	Jojoba oil, native	11078606	1
henry lamotte oils	Jojoba oil, native	5055401	1
Caelo	Walnut oil, refined	10328802	1
Caelo	Walnut oil, refined	11167103	1
Henry Lamotte Oils / No...	Flaxseed oil, native	1000000878	1
Taoasis	Macadamia oil, refined	4976601-92844	1
Caelo	Macadamia oil, refined	13012104	1
Lamotte/AHD	Evening primrose oil, refined	145581	2
Henry Lamotte /AHD	Evening primrose oil, refined	1000001044	1
Taoasis	Evening primrose oil, refined	3723-107968	1
Noweda	Evening primrose oil, refined	E1106072	1
Taoasis	Evening primrose oil, refined	12096-99883	2
Caelo	Olive oil, native	14306913	1
Caelo	Olive oil, native	15216310	2
Caelo	Olive oil, native	16212806	3
Caelo	Olive oil, native	16212801	2
Lamotte/Spangro	Olive oil, native	5891202	1
Lamotte/Spangro	Olive oil, native	5903400003	1
Bombastus	Olive oil, native	270970	3
Lamotte/Spangro	Olive oil, native	8000652001	1
Lamotte/Spangro	Olive oil, native	8001648001	1
Anzag	Olive oil, native	12077701	1
Anzag	Olive oil, native	12274104	1
Fiebig	Olive oil, native	12077702	1
Gehe	Olive oil, native	279609	1
Gehe	Olive oil, native	288752	2
HL/N/25.02.13 PZN:3649899	Olive oil, native	5283901	1
HENRY LAMOTTE OILS GmbH	Avocado oil, refined	1000001451	1
Bombastus	Olive oil, native	00270970	1
lamotte	Sesame oil, refined	123488	1
Caelo	Sesame oil, refined	13172906	6
Caelo	Sesame oil, refined	14170004	6
Caelo	Sesame oil, refined	14170005	3
Caelo	Sesame oil, refined	15374001	1
Henry Lamotte	Sesame oil, refined	5744101	1
Lamotte/Phönix	Sesame oil, refined	58772901	1
henry lamotte	Sesame oil, refined	122972	1
Henry Lamotte Oils	Sesame oil, refined	122972	1
Caelo	Sesame oil, refined	13011105	9
Caelo	Grape seed oil, refined	14127906	1
Caelo	Grape seed oil, refined	15144502	1
Caelo	Grape seed oil, refined	13065302	6
Caelo	Grape seed oil, refined	13174601	2
Caesar & Lorenz	Grape seed oil, refined	13065310	1
Caelo	Oleyl oleate (stabilised)	15321701	4
Sanacorp	Oleyl oleate (stabilised)	13378403	1
Caelo	Oleyl oleate (stabilised)	14129007	7
Sanacorp	Oleyl oleate (stabilised)	13096402	2
Caelo	Oleyl oleate (stabilised)	13096801	1
Caelo	Oleyl oleate (stabilised)	13291605	1
Sanacorp	Oleyl oleate (stabilised)	12220208	1
Noweda	Oleyl oleate (stabilised)	11/08-N03	1
Fagron	Oleyl oleate (stabilised)	11K25-N09	1
Fagron	Oleyl oleate (stabilised)	11I08-N03	1
Fagron	Oleyl oleate (stabilised)	11L08-N03	1
AHD	Oleyl oleate (stabilised)	14129003	1
Caelo	Oleyl oleate (stabilised)	14129003	1
Phoenix	Oleyl oleate (stabilised)	14129007	1
Caelo	Oleyl oleate (stabilised)	14254603	4

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Supplier	Substance	Batch	Spectra
Fagron	Oleyl oleate (stabilised)	14B14-B03-29295	1
Fagron	Oleyl oleate (stabilised)	14B14-B03-29219	1
Caelo	Oleyl oleate (stabilised)	15321706	3
Caesar&Loretz/Noweda	Oleyl oleate (stabilised)	15321702	1
Caelo	Oleyl oleate (stabilised)	15322703	2
Caesar&Loretz GmbH	Oleyl oleate (stabilised)	15410204	1
Caelo	Olive oil, native	14182305	2
Bombastus	Olive oil, native	289094	3
Bombastus	Olive oil, native	290403	7
Bombastus	Olive oil, native	287259Noweda	1
Bombastus	Olive oil, native	4328413	1
Bombastus	Olive oil, native	294035	1
Lamotte/Spangro	Olive oil, native	5671901	1
Pharmachem/AHD	Olive oil, native	13324703	1
Bombastus	Olive oil, native	277049	1
Caelo	Olive oil, native	279609	1
Sanacorp	Olive oil, native	277050	1
Sanacorp	Olive oil, native	279609	1
Bombastus	Olive oil, native	283762	2
Caelo	Olive oil, native	12388	1
Henry lamotte/N/PZN:004...	Olive oil, native	5372701	1
Fagron	Olive oil, native	15A27-B03-304709	2
Ebert & Jacobi 02.08...	Olive oil, native	15399704	1
Caesar & Loretz GmbH Hi...	Olive oil, native	16212801	1
Caesar & Loretz GmbH Hi...	Olive oil, native	16212806	1
Caelo	Olive oil, native	16144605	1
Bomastus/Phönix	Olive oil, native	302523	1
Lamotte	Olive oil, native	5903400003	1
Lamotte	Olive oil, native	8000821001	1
Henry Lamotte/Anzag	Olive oil, native	8001648001	1
Henry Lamotte Oils GmBh...	Olive oil, native	124392	1
Lamotte / Noweda	Olive oil, native	124392	1
Caelo	Olive oil, native	7031501	1
Caelo	Olive oil, native	2021502	1
Caelo	Olive oil, native	2021501	1
Caelo	Olive oil, native	7051507	1
Caelo	Olive oil, native	8121404	1
Sanacorp	Olive oil, native	1/AKD4	2
Fagron	Olive oil, native	13J25-B04-289441	1
Caelo	Olive oil, native	14024410	4
Caesar & Loretz GmbH Hi...	Olive oil, native	14182302	1
Sanacorp	Olive oil, native	14306903	1
Caesar & Loretz GmbH Hi...	Olive oil, native	15311404	1
Caelo	Olive oil, native	15363302	1
Caelo	Olive oil, native	17051403	1
Caelo	Olive oil, native	17041404	1
Caelo	Olive oil, native	18031506	1
Caelo	Olive oil, native	18041502	1
Caelo	Olive oil, native	26071403	1
Caelo	Olive oil, native	26091403	1
Caelo	Olive oil, native	23121413	1
S.Binder	Olive oil, native	284144	1
Caelo	Olive oil, native	28051405	1
Fagron	Olive oil, native	284144	2
Bombastus	Olive oil, native	287259	2
Gehe	Olive oil, native	289094	1
Gehe	Olive oil, native	289095	3
Bombastus	Olive oil, native	298007	1
Bombastus	Olive oil, native	4613M-02000	1
LAMOTTE/NOWEDA	Olive oil, native	5470202	1

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Supplier	Substance	Batch	Spectra
Bombastus	Olive oil, native	4812A-02000	1
Lamotte/Phoenix	Olive oil, native	5623601	1
Caelo	Olive oil, native	5470202	1
Anzag/Lamotte	Olive oil, native	5623601	1
Caelo	Olive oil, native	5671601	1
Caelo	Olive oil, native	5623601	1
Lamotte/Anzag	Olive oil, native	5671901	1
Henry Lamotte Oils GmbH...	Olive oil, native	5734701	1
Lamotte/Anzag	Olive oil, native	5734701	1
Lamotte / Gehe	Olive oil, native	5734701	1
Henry Lamotte/Anzag	Olive oil, native	590340003	1
Noweda	Olive oil, native	5813601	1
noweda	Olive oil, native		1
Henry Lamotte Oils GmbH	Olive oil, native	5921100001	1
Sanacorp	Olive oil, native		1
Caelo	Olive oil, native	CE834/ES	1
Bombastus	Olive oil, native	259542	1
Bombastus	Olive oil, native	256053	1
Bombastus	Olive oil, native	265359	1
Gehe	Olive oil, native	265359	1
Bombastus	Olive oil, native	266513	1
Noweda	Olive oil, native	267376	1
Bombastus	Olive oil, native	267376	2
Noweda	Olive oil, native	268118	1
Gehe	Olive oil, native	267376	1
Gehe	Olive oil, native	269674	3
Bombastus	Olive oil, native	270971	1
Gehe	Olive oil, native	272270	2
Bombastus	Olive oil, native	272270	4
Phönix 09.11.12	Olive oil, native	272270	1
Sanacorp	Olive oil, native	273659	1
Bombastus	Olive oil, native	273659	3
Gehe	Olive oil, native	274236	1
Ichthyol/Phönix	Olive oil, native	274236	1
Caelo	Olive oil, native	1031302	1
Caelo	Olive oil, native	123773	1
Caelo	Olive oil, native	4041303	1
Caelo	Olive oil, native	406212000	1
Caelo	Olive oil, native	4101312	1
Caelo	Olive oil, native	503312000	1
Caelo	Olive oil, native	6111208	1
Caelo	Olive oil, native	7071206	1
Caelo	Olive oil, native	713I-02000	1
Caelo	Olive oil, native	10111201	1
Caelo	Olive oil, native	11063901	1
Caelo	Olive oil, native	11063906	1
Caelo	Olive oil, native	11227002	2
Caelo	Olive oil, native	11227001	1
Bombastus	Olive oil, native	110816-1	1
Caelo	Olive oil, native	11227011	2
Kehr	Olive oil, native	11376906	1
Gehe	Olive oil, native	11C16-N08	1
Noweda	Olive oil, native	12077701	1
Anzag 31.10.12 ek: 2,78EUR	Olive oil, native	12077701	1
Cealo/Gehe	Olive oil, native	12077701	1
Caelo	Olive oil, native	120777027-13	1
Caelo	Olive oil, native	1207771	1
Resana GmbH	Olive oil, native	1208-3652	1
Euro OTC	Olive oil, native	1212022-01	2
Caesar & Loretz GmbH, 4...	Olive oil, native	12141306	1

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Supplier	Substance	Batch	Spectra
Phönix 28.12.12	Olive oil, native	12141305	1
Cealo/Gehe	Olive oil, native	12141306	3
Sanacorp	Olive oil, native	12141306	2
Caelo	Olive oil, native	12141308	3
Noweda	Olive oil, native	12141309	1
Cae	Olive oil, native	12141309	1
Caelo	Olive oil, native	12141310	1
Caelo	Olive oil, native	1214306	1
Caelo	Olive oil, native	12274102	3
Phönix	Olive oil, native	12274106	1
Caelo	Olive oil, native	12274108	1
Wolf Handelsgesellschaft	Olive oil, native	128972ES	1
Fagron	Olive oil, native	12A18-N08	2
Fagron	Olive oil, native	12I07-N07	3
Gehe	Olive oil, native	12I07-N07	1
Fagron	Olive oil, native	12I07-N07	1
Fagron	Olive oil, native	13010904	1
Hustadt Apotheke	Olive oil, native	13010904	1
Caelo	Olive oil, native	1301094	1
Caelo	Olive oil, native	13021410	1
Caelo	Olive oil, native	13081204	1
Alliance Healthcare	Olive oil, native	13224703	1
Fagron	Olive oil, native	13224704	2
Caelo	Olive oil, native	13224706	4
Caelo	Olive oil, native	1324704	1
Caelo	Olive oil, native	13306103	1
Caesar & Loretz GmbH	Olive oil, native	13350101	1
Phoenix	Olive oil, native	13350103	1
Caelo	Olive oil, native	13350106	4
Fagron	Olive oil, native	13c08-N06	1
Caelo	Olive oil, native	14111306	1
Caelo	Olive oil, native	141182303	1
Phoenix	Olive oil, native	1406009-01	1
J.H. Müller	Olive oil, native	140115	1
Caelo	Olive oil, native	1509212000	1
Caelo	Olive oil, native	20270912-4	1
Caelo	Olive oil, native	20061207	1
Caelo	Olive oil, native	2113Q02000	1
Caelo	Olive oil, native	24011303	1
Caelo	Olive oil, native	24011408	1
Caelo	Olive oil, native	265359	1
Gehe	Olive oil, native	275757	3
Alliance	Olive oil, native	277050	1
Gehe	Olive oil, native	278583	2
Phönix, 07.11.2011	Olive oil, native	278583	1
Gehe	Olive oil, native	281209	2
Gehe	Olive oil, native	281898	2
Gehe	Olive oil, native	284144	1
Caelo	Olive oil, native	29041301	1
Caelo	Olive oil, native	3313I-02000	1
Caelo	Olive oil, native	3212I-02000	1
Caelo	Olive oil, native	5107101	2
Henry Lamotte Oils GmbH	Olive oil, native	5107101	1
Henry Lamotte	Olive oil, native	5107101	1
Lamotte / Gehe	Olive oil, native	5127501	1
Gehe	Olive oil, native	5107101	1
HenryLamotte	Olive oil, native	5232201	2
Henry Lamotte	Olive oil, native	5232201	1
Großhandel	Olive oil, native	5232201	2
Lamotte	Olive oil, native	5232201	3

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Supplier	Substance	Batch	Spectra
H. Lamotte	Olive oil, native	5232201	1
Henry, Noweda	Olive oil, native	5232201	1
Henry Lamotte / Phoenix	Olive oil, native	5232201	1
H.Lamotte/Noweda	Olive oil, native	5232201	1
Lamotte/GH/11.09.13	Olive oil, native	5271504	1
Henry Lamotte / Phoenix	Olive oil, native	5271504	1
Henry Lamotte	Olive oil, native	5271504	1
Phönix/Lamotte	Olive oil, native	5272401	1
HenryLamotte/Phoenix	Olive oil, native	5272401	4
Lamotte Phönix	Olive oil, native	5272401	2
Henry Lamotte/Anzag	Olive oil, native	5272401	1
Caelo	Olive oil, native	5272401	2
Großhandel	Olive oil, native	5272401	1
Lamotte / Sanacorp	Olive oil, native	5283901	1
Lamotte / Gehe	Olive oil, native	5283901	2
Lamotte	Olive oil, native	5372701	1
AHD, 03.08.2011	Olive oil, native	5372701	1
Lamotte / Gehe	Olive oil, native	5372701	2
Caelo	Olive oil, native	5464901	2
Lamotte/V.d.L.	Olive oil, native	5464901	1
henry lamotte oils gmbh	Olive oil, native	5464901	1
Klenk	Olive oil, native	5470202	1
Großhandel	Olive oil, native	5470202	1
Henry Lamotte Oils Gmbh...	Olive oil, native	5470202	1
Bombastus	Olive oil, native	60081503	1
Lamotte / Gehe	Olive oil, native	L901	1
Henry Lamotte	Sesame oil, refined	124494	1
Lamotte über Sanacorp	Borage oil, refined, stabili...	125354	1
Caelo	Almond oil, refined	2101405	1
Caelo	Almond oil, refined	465957	1
Caelo	Evening primrose oil, refined	3878-124466	1
Caelo	Almond oil, refined	6031506	1
Lamotte/AHD	Evening primrose oil, refined	1000002386	1
Sanacorp	Wheatgerm oil, refined	1/AKD2	1
Henry Lamotte Oils / No...	Almond oil, refined	1000003242	1
Caelo	Peanut oil, refined	1232304	1
Caelo	Sesame oil, refined	13172908	2
Fagron	Almond oil, refined	13236411	1
Caelo	Wheatgerm oil, refined	13261603	7
Caelo	Wheatgerm oil, refined	13261604	3
Caelo	Apricot kernel oil, refined	13357604	1
Caesar & Loretz GmbH	Peanut oil, refined	13358803	1
Phönix	Peanut oil, refined	13358801	1
Fagron	Avocado oil, refined	13361406	1
Caelo	Sesame oil, refined	13397402	3
PHOENIX 15.05.2014	Borage oil, refined, stabili...	13372104	1
PHOENIX 08.05.2014	Evening primrose oil, refined	14002501	1
Caelo	Borage oil, refined, stabili...	13372110	1
Euro OTC	Evening primrose oil, refined	140133-01	1
Caelo	Wheatgerm oil, refined	14024501	5
Caelo	Wheatgerm oil, refined	14024502	1
PHOENIX 03.06.2014	Almond oil, refined	14042705	1
Caelo	Almond oil, refined	14042710	1
Caelo	Peanut oil, refined	14111401	1
Caesar & Loretz GmbH Hi...	Peanut oil, refined	14115404	1
Caelo	Almond oil, refined	141215804	1
Caelo	Grape seed oil, refined	14127902	3
Phoenix	Peanut oil, refined	14115405	1
Caelo	Sunflower oil, refined	14147101	1
Caelo	Sesame oil, refined	14170001	1

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Supplier	Substance	Batch	Spectra
Schubert / Phoenix	Sunflower oil, refined	1423F0-2027	2
AHD	Peanut oil, refined	14246901	1
Caelo	Wheatgerm oil, refined	14272514	2
Caelo	Sesame oil, refined	14351804	3
Caelo	Sunflower oil, refined	14306701	1
Sanacorp	Peanut oil, refined	14355904	1
Caesar&Loretz GmbH/Anzag	Peanut oil, refined	14355905	1
Phoenix	Peanut oil, refined	14355905	1
Euro OTC	Avocado oil, refined	150101501	1
Caelo	Almond oil, refined	15078401	1
Euro OTC	Almond oil, refined	1510014-01	1
Caelo	Almond oil, refined	15080602	1
Fischer/Gehe	Almond oil, refined	15127306	1
Caelo	Grape seed oil, refined	15144509	2
Noweda	Almond oil, refined	15197404	1
Caelo	Almond oil, refined	15197405	1
Bombastus	Almond oil, refined	15197407	1
Caelo	Sesame oil, refined	15239405	4
Caesar & Loretz/Noweda	Peanut oil, refined	15273402	1
Caelo	Sesame oil, refined	15374006	1
Caelo	Wheatgerm oil, refined	15374101	4
Caesar & Loretz/Noweda	Almond oil, refined	15409704	1
Caelo	Almond oil, refined	15409716	1
Caelo	Borage oil, refined, stabili...	16052307	2
Caelo	Almond oil, refined	15806001	1
Caesar & Loretz/Noweda	Almond oil, refined	16071002	1
Phönix	Almond oil, refined	16071006	2
Caesar & Loretz	Almond oil, refined	16071006	1
Caelo	Peanut oil, refined	16071103	1
Bombastus	Almond oil, refined	16115303	1
Bombastus	Sunflower oil, refined	281796	1
Eigenherstellung	Almond oil, refined	181114HML01	1
Eigenherstellung	Almond oil, refined	270215HJK01	1
Bombastus	Sunflower oil, refined	285243	1
PHÖNIX	Almond oil, refined	16327302	1
Eigenherstellung	Almond oil, refined	300615HML01	1
Henry Lamotte Oils/Jenn...	Sesame oil, refined	5514801	3
Bombastus	Wheatgerm oil, refined	283449	1
Lamotte	Almond oil, refined	5615001	1
lamotte noweda,	Almond oil, refined	5615001	1
Lamotte/Phoenix	Almond oil, refined	5615001	1
Lamotte / Noweda	Almond oil, refined	5615003	1
Phoenix/Lamotte	Sesame oil, refined	5634501	1
Henry Lamotte Oils GmbH	Peanut oil, refined	5699601	1
Henry Lamotte	Sunflower oil, refined	5738004	1
Lamotte über Phoenix	Sesame oil, refined	5872001	1
Noweda	Avocado oil, refined	713301202	1
Lamotte/Phoenix	Almond oil, refined	5919600001	1
Lamotte über Noweda	Sesame oil, refined	8000682001	2
Lamotte über Phoenix	Almond oil, refined	8000725001	1
Henry Lamotte/Kehr	Sesame oil, refined	8001557002	1
Audor Pharma	Evening primrose oil, refined	AP562-124	1
Caelo	Evening primrose oil, refined	AP094-115N	1
Lamotte / Gehe	Avocado oil, refined	130193	1
Henry Lamotte	Borage oil, refined, stabili...	145678	2
Henry Lamotte Oils	Borage oil, refined, stabili...	123118	1
Phönix	Borage oil, refined, stabili...	12161207	1
Sanacorp	Avocado oil, refined	713301202	1
Fagron	Avocado oil, refined	12F25-N12	1
Caelo	Borage oil, refined, stabili...	13170603	1

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Supplier	Substance	Batch	Spectra
Caelo	Borage oil, refined, stabili...	13372101	1
Caelo	Peanut oil, refined	8061303	1
Caelo	Peanut oil, refined	107063	1
Caelo	Peanut oil, refined	1224302	1
Euro OTC	Peanut oil, refined	1301015	1
Caesar&Loretz GmbH/Anzag	Peanut oil, refined	12323204	1
Caesar&Loretz GmbH/Anzag	Peanut oil, refined	13306106	1
Noweda	Peanut oil, refined	13358804	2
Caelo	Peanut oil, refined	13G30-N05	1
Caelo	Peanut oil, refined	28031304	1
Caelo	Peanut oil, refined	16011403	1
Bombastus	Almond oil, refined	273579	1
Caelo	Peanut oil, refined	5314601	1
Caelo	Peanut oil, refined	28021406	1
Caelo	Almond oil, refined	2021303	1
Eigenherstellung	Almond oil, refined	61113HML01	1
Caelo	Almond oil, refined	10131-01950	1
Caelo	Almond oil, refined	11358910	1
Caesar & Loretz/ Noweda	Almond oil, refined	12357101	2
GEHE	Almond oil, refined	13178003	1
Noweda	Almond oil, refined	13178011	2
Phönix 11.11.2013	Almond oil, refined	13236401	1
Anzag/Leyh Pharma am	Almond oil, refined	13236404	1
Caelo	Almond oil, refined	133500006	1
Caelo	Almond oil, refined	1335006	1
Eigenherstellung	Almond oil, refined	240513HML01	1
Phoenix/Lamotte	Almond oil, refined	5214206	1
Noweda/Lamotte Oils	Almond oil, refined	5214206	1
Bombastus	Almond oil, refined	274565	1
Lamotte/GEHE	Almond oil, refined	5269301	3
Lamotte/Noweda	Almond oil, refined	5438302	1
Phönix/Lamotte	Almond oil, refined	5438302	2
Lamotte	Almond oil, refined	548302	1
Taoasis	Almond oil, refined	5511701-113571	1
Caelo	Almond oil, refined	0-240513-1	1
Phönix	Evening primrose oil, refined	12325105	1
Caelo	Evening primrose oil, refined	1312816	1
Fagron	Evening primrose oil, refined	13E06-No9	1
Phoenix	Evening primrose oil, refined	14002503	1
Lamotte	Sesame oil, refined	123488	1
Euro OTC	Sesame oil, refined	1205407	1
Caelo	Sesame oil, refined	11224108	3
Caelo	Sesame oil, refined	12054501	1
Phönix 12.12.12	Sesame oil, refined	12054508	1
Caelo	Sesame oil, refined	12054508	4
Caelo	Sesame oil, refined	13011104	4
Caelo	Sesame oil, refined	13011107	7
Caelo	Sesame oil, refined	13011109	1
Henry Lamotte Oils	Sesame oil, refined	5319201	2
Caelo	Sesame oil, refined	25051305	1
Bombastus	Sunflower oil, refined	274107	2
Caelo	Sunflower oil, refined	12009804	2
Caelo	Grape seed oil, refined	12149204	4
Caelo	Grape seed oil, refined	12149205	1
Caelo	Grape seed oil, refined	13065309	4
Caelo	Walnut oil, refined	13338302	1
Caelo	Wheatgerm oil, refined	12220306	2
Caelo	Wheatgerm oil, refined	12220304	2
Caelo	Wheatgerm oil, refined	12220307	1
Caelo	Wheatgerm oil, refined	13011502	1

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Supplier	Substance	Batch	Spectra
Caelo	Wheatgerm oil, refined	13011501	4
Caelo	Wheatgerm oil, refined	13011505	7
Caelo	Wheatgerm oil, refined	13011507	3
Euro OTC	Wheatgerm oil, refined	1305015-01	1
Fagron	Wheatgerm oil, refined	13D22-N13	1
Caelo	Wheatgerm oil, refined	W-240513-2	1
Caelo	Rapeseed oil, refined	12054406	2
Fagron	Rapeseed oil, refined	13011003	1
Euro OTC	Sesame oil, refined	124494	1
Caelo	Sesame oil, refined	10011503	1
Caelo	Sesame oil, refined	11081513	1
Henry Lamotte / Noweda	Sesame oil, refined	5639301	1
Henry Lamotte Oils GmbH.	Sesame oil, refined	5639301	1
Lamotte über Phoenix	Sesame oil, refined	5639301	2
Lamotte über Phoenix	Sesame oil, refined	5872901	2
Noweda/Henry Lamotte Oils	Sesame oil, refined	5872901	1
Lamotte über Phoenix	Sesame oil, refined	5821001	1
Henry Lamotte	Sesame oil, refined	5872901	1
Lamotte über Noweda	Sesame oil, refined	1000002705	1
Henry Lamotte Oils GmbH	Sesame oil, refined	122972	1
Gehe	Sesame oil, refined	122972	1
Gehe / 23.01.13 Henry L...	Sesame oil, refined	122972	1
Lamotte/ Noweda	Sesame oil, refined	123488	1
Henry Lamotte/ 26.06.13...	Sesame oil, refined	123488	1
Henry Lamotte Oils GmbH	Sesame oil, refined	123488	1
Lamotte	Sesame oil, refined	123826	1
Henry Lamotte	Sesame oil, refined	123826	1
Henr	Sesame oil, refined	123826	1
Caelo	Sesame oil, refined	123826	1
Caelo	Sesame oil, refined	10241803	1
Caelo	Sesame oil, refined	11224103	1
Caelo	Sesame oil, refined	1205408	1
Caelo	Sesame oil, refined	1301105	1
Euro OTC	Sesame oil, refined	13011107	1
Caelo	Sesame oil, refined	14101302	1
Caelo	Sesame oil, refined	17011405	1
Caelo	Sesame oil, refined	21051305	1
Caelo	Sesame oil, refined	30051201	1
Lamotte	Sesame oil, refined	4711A-02016	1
HenryLamotte/Phoenix	Sesame oil, refined	5135601	1
Henry Lamotte	Sesame oil, refined	5319201	1
Lamotte/Krieger	Sesame oil, refined	5319201	1
Caelo	Sesame oil, refined	5319201	1
Euro OTC	Soy lecithin, liquid	1404022-01	1
Euro OTC	Soy lecithin, liquid	1404022V-02	1
Euro OTC	Soy lecithin, liquid	1503038	1
Euro OTC	Soy lecithin, liquid	1204028-01	1
Euro OTC	Soy lecithin, liquid	14404022-01	1
Euro OTC	Soy lecithin, liquid	20061209	1
Caelo	Soy oil, refined	14194107	1
Euro OTC	Soy lecithin, liquid	1305019-01	1
Euro OTC	Soy lecithin, liquid	614E3336	1
Wolf Handelsgesellschaft	Sunflower oil, refined	1822313	1
Henry Lamotte/Sanacorp	Sunflower oil, refined	5738004	1
Bombastus	Sunflower oil, refined	271457	1
Bombastus	Sunflower oil, refined	259035	1
Henry Lamotte	Sunflower oil, refined	8001230001	1
Caelo	Sunflower oil, refined	11000605	2
Wolf Handelsgesellschaft	Sunflower oil, refined	1692305SK	1
Bombastus	Sunflower oil, refined	275830	1

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Supplier	Substance	Batch	Spectra
Gehe	Sunflower oil, refined	11126606	1
J.H. Müller	Sunflower oil, refined	140229	1
Lamotte/L3	Sunflower oil, refined	5422401	1
Noweda / Henry Lamotte	Sunflower oil, refined	5422401	1
Cealo	Grape seed oil, refined	15144505	1
Caelo	Grape seed oil, refined	14214606	1
Fagron	Grape seed oil, refined	16092401	1
Caelo	Grape seed oil, refined	10222901	1
Caelo	Grape seed oil, refined	12149211	1
Caelo	Grape seed oil, refined	12149210	1
Caelo	Grape seed oil, refined	12149212	2
Caelo	Grape seed oil, refined	12149203	1
Holdermann	Grape seed oil, refined	12149212	1
Gehe	Grape seed oil, refined	12149204	1
Hepart AG	Walnut oil, refined	12214904	1
Caelo	Walnut oil, refined	12214904	1
Caelo	Walnut oil, refined	12214902	1
Caelo	Walnut oil, refined	13202401	3
Voegelé	Walnut oil, refined	2013113013	2
Caelo	Walnut oil, refined	24101309	1
Caelo	Wheatgerm oil, refined	5011502	1
Caelo	Wheatgerm oil, refined	13261601	5
Caelo	Wheatgerm oil, refined	14272511	2
Caelo	Wheatgerm oil, refined	14356001	4
Noweda	Wheatgerm oil, refined	14356003	1
Caelo	Wheatgerm oil, refined	14356003	1
Caelo	Wheatgerm oil, refined	14356006	3
Caelo	Wheatgerm oil, refined	14366001	1
Caelo	Wheatgerm oil, refined	15111602	2
Caelo	Wheatgerm oil, refined	15111603	1
Caelo	Wheatgerm oil, refined	15111605	1
Phoenix	Wheatgerm oil, refined	15374101	1
Caelo	Wheatgerm oil, refined	15374104	1
Phoenix	Wheatgerm oil, refined	16137403	1
Bombastus	Wheatgerm oil, refined	286986	1
Caelo	Wheatgerm oil, refined	15406206	1
Bombastus	Wheatgerm oil, refined	289212	1
Caelo	Wheatgerm oil, refined	292513	1
phönix	Wheatgerm oil, refined		1
Caelo	Wheatgerm oil, refined	213E-02784	1
Primavera	Wheatgerm oil, refined	3606132	1
Caelo	Wheatgerm oil, refined	11227305	2
Ichthyl Phönix	Wheatgerm oil, refined	12220302	1
Großhandel	Wheatgerm oil, refined	12220302	1
Caelo	Wheatgerm oil, refined	12220305	1
Caelo	Wheatgerm oil, refined	13011503	2
Caelo	Wheatgerm oil, refined	13011508	2
Caelo	Wheatgerm oil, refined	13261605	1
Caelo	Wheatgerm oil, refined	14272513	1

- 53 053 spectra from 332 *Apo-Ident* customers from a total of 18 529 batches from a further 306 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 *Triglycerides* 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 *Triglycerides* 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	3180	0	31 164
Type B	0	3254	88	59 730
Type C	0	5274	114	52 775

The substance/substance group *Triglycerides* 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 % (> 99.9688 %)	100.0000 % (> 99.8113 %)
Type B	100.0000 % (> 99.9717 %)	97.3668 % (> 97.2771 %)
Type C	100.0000 % (> 99.6026 %)	97.8842 % (> 97.8285 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30647	31350	1.94	46.79
30679	31729	2.57	84.37
30754	31496	6.87	33.53
30840	33060	4.44	31.09
30855	31708	2.54	68.86
30863	31496	8.71	33.24
30873	31215	4.73	46.68
30878	31361	5.88	70.36
30981	30981	0.00	65.74
31016	31016	0.00	55.51
31034	31523	0.93	31.48
31121	31121	0.00	61.37
31122	31122	0.00	21.54
31156	31156	0.00	34.84
31161	31161	0.00	62.00
31172	31172	0.00	73.08

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31178	31729	4.88	86.35
31210	31210	0.00	57.69
31215	31215	0.00	47.81
31216	31216	0.00	65.33
31217	31217	0.00	53.38
31246	31246	0.00	32.38
31250	31250	0.00	28.64
31274	31274	0.00	52.25
31322	31322	0.00	42.20
31326	33064	5.01	76.40
31332	31332	0.00	49.71
31336	31336	0.00	34.54
31337	31770	1.99	36.44
31344	31274	2.15	52.58
31346	31801	1.86	32.84
31350	31350	0.00	45.02
31356	32195	1.41	34.03
31361	31361	0.00	66.80
31362	30981	4.74	62.98
31374	31274	2.04	51.99
31375	31375	0.00	27.55
31376	31350	2.82	45.03
31378	31491	4.00	55.32
31380	31216	2.35	64.40
31382	31382	0.00	40.98
31384	31161	2.96	62.45
31460	31460	0.00	65.90
31482	31322	1.52	41.87
31491	31491	0.00	54.21
31496	31496	0.00	32.97
31519	31322	3.02	41.73
31523	31523	0.00	28.73
31540	31729	2.97	85.35
31572	31572	0.00	64.96
31584	31382	1.19	41.02
31585	31801	3.30	35.40
31589	31572	2.81	65.97
31609	31609	0.00	51.09
31616	31156	2.36	34.89
31662	31801	2.40	33.30
31677	31361	7.28	68.56
31708	31708	0.00	65.29
31729	31729	0.00	84.09
31745	31833	7.14	19.19
31770	31770	0.00	36.27
31775	31775	0.00	66.97
31792	31729	0.96	82.74
31801	31801	0.00	33.65
31825	31361	5.62	65.42
31833	31833	0.00	17.72
31834	31016	4.63	58.08
31875	31729	7.74	85.33
32195	32195	0.00	32.41

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Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
32680	32680	0.00	32.95
32683	32683	0.00	28.23
32730	31210	2.05	57.48
32745	31217	3.23	52.24
32989	30981	6.27	61.43
33059	33059	0.00	31.28
33060	33060	0.00	31.31
33064	33064	0.00	71.84
33067	33067	0.00	33.01
33070	33070	0.00	38.11

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Triglycerides, medium-chain
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31483-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Triglycerides, medium-chain; Oleum neutrale; Triglycerida saturada media

Special notes

When selecting the *Triglycerides, medium-chain* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Triglycerides, medium-chain*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Triglycerides, m...	13392404	31483	40	AR-14-FG-012976-01
Caelo	Triglycerides, m...	13348507	31484	40	20131028
Euro OTC	Triglycerides, m...	1402019-01	31485	40	20140317
Euro OTC	Triglycerides, m...	1509022	31771	40	20151007*
Euro OTC	Triglycerides, m...	1511011	31804	40	20151125*
Euro OTC	Triglycerides, m...	1601050	31955	40	20160218*

Validation samples

A total of 156 379 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 *Triglycerides, medium-chain*. These samples are listed above in the [calibration samples](#) section.
- 34 104 spectra from a total of 792 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 360 spectra of 12 reference samples from the substance/substance group *Triglycerides, medium-chain*.

Supplier	Substance	Batch	Sample ID	Spectra
zu erfassen	Triglycerides, medium-chain	pending	30174	40
Caelo	Triglycerides, medium-chain	13392404	31483 [†]	20
Caelo	Triglycerides, medium-chain	13348507	31484 [†]	20
Euro OTC	Triglycerides, medium-chain	1402019-01	31485 [†]	20
Euro OTC	Triglycerides, medium-chain	1509022	31771 [†]	20
Euro OTC	Triglycerides, medium-chain	1511011	31804 [†]	20
Euro OTC	Triglycerides, medium-chain	1601050	31955 [†]	20
Caelo	Triglycerides, medium-chain	161243	32204	40
Euro OTC	Triglycerides, medium-chain	1603041	32278	40
Euro OTC	Triglycerides, medium-chain	1606035	32464	40
Caelo	Triglycerides, medium-chain	162385	32697	40
Caelo	Triglycerides, medium-chain	170160	33077	40

- 63 234 spectra from a total of 1466 batches from further 439 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*

*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.

[†]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*.

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.

- 672 spectra from 218 *Apo-Ident* customers from 189 batches from the substance/substance group *Triglycerides, medium-chain*.

Supplier	Substance	Batch	Spectra
Bionorica ethics	Triglycerides, medium-chain	91713	2
Bionorica	Triglycerides, medium-chain	91719	2
THC/Noweda	Triglycerides, medium-chain	93572	1
Caelo	Triglycerides, medium-chain	11301106	14
Sanacorp	Triglycerides, medium-chain	93574	1
Caelo	Triglycerides, medium-chain	14098306	4
Caelo	Triglycerides, medium-chain	14219003	6
Sanacorp	Triglycerides, medium-chain	14219003	3
Caelo	Triglycerides, medium-chain	14219007	5
Caelo	Triglycerides, medium-chain	14219009	6
Caelo	Triglycerides, medium-chain	14380802	8
Caelo	Triglycerides, medium-chain	14380803	7
Caelo	Triglycerides, medium-chain	14380804	11
Fagron	Triglycerides, medium-chain	14G25-B03	3
Fagron	Triglycerides, medium-chain	14G25B03	1
Fagron	Triglycerides, medium-chain	14G25-B03-302294	4
Euro OTC	Triglycerides, medium-chain	1504029-02	3
Euro OTC	Triglycerides, medium-chain	1509022-01	2
Caelo	Triglycerides, medium-chain	15139605	4
Phoenix	Triglycerides, medium-chain	15139605	1
Miglyol	Triglycerides, medium-chain	15139605	1
Caelo	Triglycerides, medium-chain	15139607	9
Caelo	Triglycerides, medium-chain	15139608	12
Caelo	Triglycerides, medium-chain	15272003	8
Caelo	Triglycerides, medium-chain	15270004	1
/Sanacorp 02.05.2016	Triglycerides, medium-chain	15272004	1
Caelo	Triglycerides, medium-chain	15272004	18
Caelo	Triglycerides, medium-chain	15272005	5
Caelo	Triglycerides, medium-chain	15272006	9
Caelo	Triglycerides, medium-chain	15272007	3
Caelo	Triglycerides, medium-chain	15379608	4
Caelo	Triglycerides, medium-chain	15379609	1
Caesar & Loretz GmbH Hi...	Triglycerides, medium-chain	15379610	1
Ebert 12.10.16	Triglycerides, medium-chain	15379611	1
Euro OTC	Triglycerides, medium-chain	1601050-01	7
Caelo	Triglycerides, medium-chain	1572006	1
THC Pharm	Triglycerides, medium-chain		1
Caelo	Triglycerides, medium-chain	2014030260	1
THC/Sana	Triglycerides, medium-chain	2015070139	2
Caelo	Triglycerides, medium-chain	6061201	1
Sanacorp	Triglycerides, medium-chain	58/AKD4	1
THC/Noweda	Triglycerides, medium-chain	91714	1
v.d.l	Triglycerides, medium-chain	10356201	1
Noweda	Triglycerides, medium-chain	11207501	1
Caelo	Triglycerides, medium-chain	10356205	1
Fagron	Triglycerides, medium-chain	110321	1
Fiebig	Triglycerides, medium-chain	11207502	1
Caelo	Triglycerides, medium-chain	11207501	1
Caelo	Triglycerides, medium-chain	11207502	2

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Supplier	Substance	Batch	Spectra
Caelo	Triglycerides, medium-chain	11301105	1
Phönix	Triglycerides, medium-chain	11301106	1
Caelo	Triglycerides, medium-chain	12078603	13
Fagron	Triglycerides, medium-chain	11L19-N20	1
Caelo	Triglycerides, medium-chain	27101202	1
Fagron	Triglycerides, medium-chain	12A20-N16	2
Caelo	Triglycerides, medium-chain	13081205	1
Caelo	Triglycerides, medium-chain	11031502	1
Bionorica	Triglycerides, medium-chain	87113	1
Caelo	Triglycerides, medium-chain	6051503	1
Caelo	Triglycerides, medium-chain	13348501	3
Gehe	Triglycerides, medium-chain	14D23-B02-293330	1
Fagron	Triglycerides, medium-chain	14G25-B03-296937	4
Sanacorp	Triglycerides, medium-chain	56/AKD3	1
Sanacorp/Bionorica Ethics	Triglycerides, medium-chain	83204	1
Phönix 07.11.12	Triglycerides, medium-chain	58447	1
Bionorica Ethics	Triglycerides, medium-chain	62424	1
Bionorica/Phoenix	Triglycerides, medium-chain	58448	11
Bionorica	Triglycerides, medium-chain	79406	1
Caelo	Triglycerides, medium-chain	1115805	1
Caelo	Triglycerides, medium-chain	2101305	1
Fagron	Triglycerides, medium-chain	101001	1
Caelo	Triglycerides, medium-chain	8011301	1
Caelo	Triglycerides, medium-chain	11154601	1
Apotheke in Steinkuhl	Triglycerides, medium-chain	101110	1
Caelo	Triglycerides, medium-chain	11207503	1
Caelo	Triglycerides, medium-chain	11301109	3
Caesar & Loretz GmbH	Triglycerides, medium-chain	12078603	1
Caelo	Triglycerides, medium-chain	12078604	12
Caelo	Triglycerides, medium-chain	12078605	4
gehe, 23.01.2013	Triglycerides, medium-chain	12078604	1
Euro OTC	Triglycerides, medium-chain	1210002-01	5
Caelo	Triglycerides, medium-chain	12101303	1
Caelo	Triglycerides, medium-chain	1225604	1
Caelo	Triglycerides, medium-chain	1225605	1
Caelo	Triglycerides, medium-chain	12256504	6
Caelo	Triglycerides, medium-chain	12256505	22
Phönix	Triglycerides, medium-chain	12256505	1
Noveda	Triglycerides, medium-chain	12256505	1
Gehe	Triglycerides, medium-chain	12256505	1
Caelo	Triglycerides, medium-chain	1226505	1
Gehe 06.05.2013	Triglycerides, medium-chain	12256505	1
Caelo	Triglycerides, medium-chain	1235601	1
Caelo	Triglycerides, medium-chain	12356901	6
Phönix	Triglycerides, medium-chain	12356901	2
Caelo	Triglycerides, medium-chain	12356903	11
Caelo	Triglycerides, medium-chain	12356904	1
Caelo	Triglycerides, medium-chain	12356908	22
Caelo	Triglycerides, medium-chain	12356909	4
Caelo	Triglycerides, medium-chain	1256505	1
Fagron	Triglycerides, medium-chain	12I04-N07	8
Fagron	Triglycerides, medium-chain	12K07-N22	4
Caelo	Triglycerides, medium-chain	13095304	9
celo/phönix	Triglycerides, medium-chain	13095306	1
Caelo	Triglycerides, medium-chain	13095306	2
Caelo	Triglycerides, medium-chain	13098601	12
Großhandel	Triglycerides, medium-chain	13098601	1
Ebert	Triglycerides, medium-chain	13098601	1
Caelo	Triglycerides, medium-chain	13098605	6
Caelo	Triglycerides, medium-chain	13177101	8

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Supplier	Substance	Batch	Spectra
Phönix	Triglycerides, medium-chain	13177102	1
Gehe	Triglycerides, medium-chain	13177102	3
Caelo	Triglycerides, medium-chain	13177102	23
Caesar&loretz,Phoenix	Triglycerides, medium-chain	13177102	1
Caelo	Triglycerides, medium-chain	13348502	6
Sanacorp	Triglycerides, medium-chain	13348502	2
Caelo	Triglycerides, medium-chain	13348503	8
Caelo	Triglycerides, medium-chain	13348506	4
Caelo	Triglycerides, medium-chain	13348507	1
Fagron	Triglycerides, medium-chain	13E24-N04	13
Fagron	Triglycerides, medium-chain	13H02N03	1
Caelo	Triglycerides, medium-chain	1803111	2
Caelo	Triglycerides, medium-chain	18111309	1
HCT Pharma	Triglycerides, medium-chain	2012100833	1
Caelo	Triglycerides, medium-chain	18031307	1
Caelo	Triglycerides, medium-chain	31051303	1
Caelo	Triglycerides, medium-chain	2113Q01998	1
Caelo	Triglycerides, medium-chain	20270312-3	1
Euro OTC	Triglycerides, medium-chain	58448	2
Caelo	Triglycerides, medium-chain	4110i-01998	1
Bionorica	Triglycerides, medium-chain	69719	2
Euro OTC	Triglycerides, medium-chain	67940	2
EuRho	Triglycerides, medium-chain	4121201	1
Euro OTC	Triglycerides, medium-chain	1105005-01	2
Caelo	Triglycerides, medium-chain	614M1998	1
Euro OTC	Triglycerides, medium-chain	1111037-01	3
EuRho	Triglycerides, medium-chain	1111037-01	1
Phönix Gotha	Triglycerides, medium-chain	1111037-01	1
Caesar/Noweda	Triglycerides, medium-chain	11301104	1
anzag, 20.11.2012	Triglycerides, medium-chain	11L19-N20	2
Phönix Gotha	Triglycerides, medium-chain	1205015-01	2
Euro OTC	Triglycerides, medium-chain	1205015-01	2
Fagron	Triglycerides, medium-chain	1210002-01	3
Phönix Gotha	Triglycerides, medium-chain	1210002-01	2
phönix 22.01.2013	Triglycerides, medium-chain	1210002-01	1
Caelo	Triglycerides, medium-chain	1210002-01	4
Phönix	Triglycerides, medium-chain	1210002-01	2
Phönix Gotha	Triglycerides, medium-chain	1302004-01	3
Euro OTC	Triglycerides, medium-chain	130200401	1
Eurho/Phoenix	Triglycerides, medium-chain	13095303	2
Euro OTC	Triglycerides, medium-chain	1302004-01	10
Caesar/Noweda	Triglycerides, medium-chain	13177109	1
Hansen&Rosenthal/Phönix	Triglycerides, medium-chain	1406016-01	1
Phönix Gotha	Triglycerides, medium-chain	1411009-01	2
Phönix Gotha	Triglycerides, medium-chain	1411009-02	1
Euro OTC	Triglycerides, medium-chain	1411009-02	2
Caelo	Triglycerides, medium-chain	150402902	1
Caelo	Triglycerides, medium-chain	15012016	1
Euro OTC	Triglycerides, medium-chain	1511011-01	6
Phönix Gotha	Triglycerides, medium-chain	1504029-01	2
Caelo	Triglycerides, medium-chain	3413I-01998	1
Caelo	Triglycerides, medium-chain	1537908	1
Caelo	Triglycerides, medium-chain	50775165	1
Caelo	Triglycerides, medium-chain		2
Pharimex	Triglycerides, medium-chain	75316	2
Euro OTC	Triglycerides, medium-chain	1411009-01	5
Caelo	Triglycerides, medium-chain	15139604	1
Caelo	Triglycerides, medium-chain	15272008	1
Fagron	Triglycerides, medium-chain	15H03-B03-312351	2
Caelo	Triglycerides, medium-chain	1539605	1

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Supplier	Substance	Batch	Spectra
Euro OTC	Triglycerides, medium-chain	1603041-02	2
Euro OTC	Triglycerides, medium-chain	2614A-01998	1
Sanacorp	Triglycerides, medium-chain	12356903	1
Bionorica Ethics/AHD	Triglycerides, medium-chain	62424	2
Sanacorp	Triglycerides, medium-chain	12356908	1
BionoricPhoenix	Triglycerides, medium-chain	958448	1
Bionorica	Triglycerides, medium-chain	87112	2
THC Pharm/Sanacorp	Triglycerides, medium-chain	91714	1
Bionorica/Noweda	Triglycerides, medium-chain	93566	1
Fagron	Triglycerides, medium-chain	12/04-N07	1
EuRho/Phönix	Triglycerides, medium-chain	1411009-02	1
Fagron	Triglycerides, medium-chain	14D11-N01	1
Fagron	Triglycerides, medium-chain	14G25-B03-305014	1
Euro OTC	Triglycerides, medium-chain	1504029-01	5
Fagron	Triglycerides, medium-chain	14K28-N01	1
Anzag/Henry Lamotte	Triglycerides, medium-chain	1504029-02	1
Caelo	Triglycerides, medium-chain	15080603	1
Hansen & Rosenthal/Noweda	Triglycerides, medium-chain	1509022-01	1
Euro OTC	Triglycerides, medium-chain	151101101	1
Bombastus	Triglycerides, medium-chain	15139608	1
Fagron	Triglycerides, medium-chain	15D24-B03	1
Fagron	Triglycerides, medium-chain	15D24-B03-307759	1
Fagron	Triglycerides, medium-chain	15H03-B03-312924	5
Fagron	Triglycerides, medium-chain	15H03-B03-318529	1
Fagron	Triglycerides, medium-chain	15H03-B03-325574	2
Fagron	Triglycerides, medium-chain	15H03-B03-525120	3
Cremer Oleo GmbH & Co K...	Triglycerides, medium-chain	15H03-B03-525120	1
Fagron	Triglycerides, medium-chain	15H03-B03-525189	1
Fagron	Triglycerides, medium-chain	15H03-B03-525271	1
Gehe	Triglycerides, medium-chain	1601050-01	1
Euro OTC	Triglycerides, medium-chain	160105001	1
GEHE	Triglycerides, medium-chain	1603041-01	1
Anzag	Triglycerides, medium-chain	12078604	2
Gehe	Triglycerides, medium-chain	1603041-02	1
Euro OTC	Triglycerides, medium-chain	41141312	1
Anzag	Triglycerides, medium-chain	12256505	1
Gehe	Triglycerides, medium-chain	1302004-01	2
Caelo	Triglycerides, medium-chain	613A-01998	1
Euro OTC	Triglycerides, medium-chain	1007009-01	1
Caelo	Triglycerides, medium-chain	101001	1
Noweda	Triglycerides, medium-chain	101001	1
Fagron	Triglycerides, medium-chain	10K09-0031	1
Caelo	Triglycerides, medium-chain	10356208	1
Caelo	Triglycerides, medium-chain	11154602	2
Anzag 11.10.12	Triglycerides, medium-chain	11301109	1
Fagron	Triglycerides, medium-chain	11C22-N03	1
Caelo	Triglycerides, medium-chain	11D29-N01	1
Phönix	Triglycerides, medium-chain	11320508	1
Fagron	Triglycerides, medium-chain	11G28-N07	1
Eurho	Triglycerides, medium-chain	1205015-01	1
Fagron	Triglycerides, medium-chain	120604	1
Gehe	Triglycerides, medium-chain	12078603	1
Phönix 29.10.12	Triglycerides, medium-chain	12078604	1
Caelo	Triglycerides, medium-chain	12253802	5
Fagron	Triglycerides, medium-chain	12104-N07	1
EuRho/Phönix	Triglycerides, medium-chain	13020004-02	1
Gehe	Triglycerides, medium-chain	1302004	1
Caelo	Triglycerides, medium-chain	1302004-01	1
Henry Lamotte	Triglycerides, medium-chain	1302004-01	1
Euro OTC	Triglycerides, medium-chain	1302004-02	5

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Supplier	Substance	Batch	Spectra
Phönix Gotha	Triglycerides, medium-chain	1302004-02	1
Sanacorp	Triglycerides, medium-chain	130502	1
Alliance Healthcare	Triglycerides, medium-chain	1302004-02	1
Fagron	Triglycerides, medium-chain	130502	1
Gehe	Triglycerides, medium-chain	1309025-01	1
Euro OTC	Triglycerides, medium-chain	1309025-01	1
Phoenix	Triglycerides, medium-chain	13098601	1
Caesar & Loretz GmbH	Triglycerides, medium-chain	13098601	1
Sanacorp	Triglycerides, medium-chain	13177102	1
	Triglycerides, medium-chain	13E24-N04	3
Phönix 11.11.2014	Triglycerides, medium-chain	13E2-N04	1
Fagron	Triglycerides, medium-chain	13H02-N03	1
Fagron	Triglycerides, medium-chain	13J21-N06	1
Fagron	Triglycerides, medium-chain	13j25-b11	1
Euro OTC	Triglycerides, medium-chain	1402019-01	1
Euro OTC	Triglycerides, medium-chain	141100901	1
Fagron	Triglycerides, medium-chain	14D08-N01	1
Caesar&lorenz,Phoenix	Triglycerides, medium-chain	14219003	1
Caelo	Triglycerides, medium-chain	14K28-N01	1
Euro OTC	Triglycerides, medium-chain	150902201	1
Caelo	Triglycerides, medium-chain	3113506	3
Caelo	Triglycerides, medium-chain	AKD5	1
THC Pharma	Triglycerides, medium-chain	2012050379	1
Fagron	Triglycerides, medium-chain	Ch120604	1
endima	Triglycerides, medium-chain	112k04	1
Caelo	Triglycerides, medium-chain	60492256	1

- 57 769 spectra from 332 *Apo-Ident* customers from a total of 19 905 batches from a further 328 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 *Triglycerides, medium-chain* 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 *Triglycerides, medium-chain* 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	34 104
Type B	0	350	10	63 234
Type C	0	661	11	57 769

The substance/substance group *Triglycerides, medium-chain* 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 % (> 99.9690 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9710 %)	97.2222 % (> 96.3889 %)
Type C	100.0000 % (> 99.5963 %)	98.3631 % (> 97.9167 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31483	31483	0.00	22.86
31484	31804	1.83	19.76
31485	31804	2.05	19.85
31771	31771	0.00	21.67
31804	31804	0.00	19.16
31955	31955	0.00	20.49

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Triglycerol diisostearate
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30756-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Triglycerol diisostearate; Triglycerinum diisostearinicum; Triglyceroli diisostearas

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Triglycerol diisostearate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Triglycerol diis...	12018503	30756	40	20120201
Caelo	Triglycerol diis...	13081002	31219	40	1403749
Caelo	Triglycerol diis...	14118801	31338	40	20140425

Validation samples

A total of 156 379 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 *Triglycerol diisostearate*. These samples are listed above in the [calibration samples](#) section.
- 34 224 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 80 spectra of 2 reference samples from the substance/substance group *Triglycerol diisostearate*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Triglycerol diisostearate	12018501	30568	40
Caelo	Triglycerol diisostearate	163311	33094	40

- 63 514 spectra from a total of 1475 batches from further 439 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.

- 59 spectra from 44 *Apo-Ident* customers from 20 batches from the substance/substance group *Triglycerol diisostearate*.

Supplier	Substance	Batch	Spectra
Caelo	Triglycerol diisostearate	14193003	3
Caelo	Triglycerol diisostearate	13081002	4
Caelo	Triglycerol diisostearate	12359401	3
Caelo	Triglycerol diisostearate	13399003	4
Caelo	Triglycerol diisostearate	14054802	2
gehe	Triglycerol diisostearate	14054802	1

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Supplier	Substance	Batch	Spectra
Gehe	Triglycerol diisostearate	14118801	1
Audor Pharma	Triglycerol diisostearate	14118801	1
Caelo	Triglycerol diisostearate	14118801	3
Caelo	Triglycerol diisostearate	14118804	1
Caelo	Triglycerol diisostearate	14193008	3
Caelo	Triglycerol diisostearate	14380504	6
Noweda	Triglycerol diisostearate	14193008	1
Caelo	Triglycerol diisostearate	15137505	4
Caelo	Triglycerol diisostearate	15283404	2
Caelo	Triglycerol diisostearate	16062502	2
Caelo	Triglycerol diisostearate	11162902	1
Caelo	Triglycerol diisostearate	15283402	1
Caelo	Triglycerol diisostearate	12018503	2
Caelo	Triglycerol diisostearate	12018501	1
Caelo	Triglycerol diisostearate	12133303	3
Gehe	Triglycerol diisostearate	12359401	1
Caelo	Triglycerol diisostearate	12359405	4
Caelo	Triglycerol diisostearate	13236704	3
Caelo	Triglycerol diisostearate	11074801	1
Phoenix	Triglycerol diisostearate	14054802	1

- 58 382 spectra from 332 *Apo-Ident* customers from a total of 20 073 batches from a further 328 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 *Triglycerol diisostearate* 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 *Triglycerol diisostearate* 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	34 224
Type B	0	80	0	63 514
Type C	0	58	1	58 382

The substance/substance group *Triglycerol diisostearate* 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 % (> 99.9691 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.5964 %)	98.3051 % (> 93.2203 %)

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

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

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30756	31219	5.89	40.53
31219	31219	0.00	45.32
31338	31219	6.71	44.74

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Verbena oil, nature-identical
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30666-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Verbena oil, nature-identical; Oleum verbenae

Special notes

When selecting the *Verbena oil, nature-identical* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Verbena oil, nature-identical*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Verbena oil, nat...	10368808	30666	40	20101229
Caelo	Verbena oil, nat...	13141710	31194	40	1412074
Caelo	Verbena oil, nat...	14026003	31399	40	20140128
Caelo	Verbena oil, nat...	15229809	32071	40	20150714

Validation samples

A total of 156 379 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 *Verbena oil, nature-identical*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 794 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 20 spectra of 1 reference samples from the substance/substance group *Verbena oil, nature-identical*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Verbena oil, nature-identical	15229809	32071 [†]	20

- 63 574 spectra from a total of 1476 batches from further 439 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 *Verbena oil, nature-identical*.

Supplier	Substance	Batch	Spectra
Caelo	Verbena oil, nature-identical	13141704	1

[†]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*.

- 58 440 spectra from 332 *Apo-Ident* customers from a total of 20 091 batches from a further 328 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 *Verbena oil, nature-identical* 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 *Verbena oil, nature-identical* 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	34 184
Type B	0	20	0	63 574
Type C	0	1	0	58 440

The substance/substance group *Verbena oil, nature-identical* 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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9712 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.6053 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30666	31194	2.29	57.53
31194	31194	0.00	59.92
31399	31194	3.43	59.06
32071	31194	4.46	56.78

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Viscous base solution (NRF p.20.)
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30659-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Viscous base solution (NRF p.20.)

Special notes

When selecting the *Viscous base solution (NRF p.20.)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Viscous base solution (NRF p.20.)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Viscous base sol. ...	12127301	30659	40	1403145
Caelo	Viscous base sol. ...	14020401	31354	40	20140124
Caelo	Viscous base sol. ...	14109401	31658	40	AR-15-FG-007904-01
Caelo	Viscous base sol. ...	15265401	31790	40	20150825
Caelo	Viscous base sol. ...	153888	31884	40	20151124*
Caelo	Viscous base sol. ...	153889	31886	40	20151124*

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Viscous base sol...	154121	31887	40	20151130*
Caelo	Viscous base sol...	153890	31890	40	20151124*
Caelo	Viscous base sol...	153894	31893	40	20151130*
Caelo	Viscous base sol...	153895	31896	40	20151130*
Caelo	Viscous base sol...	153896	31897	40	20151130*
Caelo	Viscous base sol...	153897	31900	40	20151130*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 480 spectra of 12 reference samples from the substance/substance group *Viscous base solution* (NRF p.20.). These samples are listed above in the [calibration samples](#) section.
- 33 864 spectra from a total of 786 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 1760 spectra of 44 reference samples from the substance/substance group *Viscous base solution* (NRF p.20.).

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Viscous base solution (NRF p...	10160601	30161	40
Caelo	Viscous base solution (NRF p...	10232201	30167	40
Caelo	Viscous base solution (NRF p...	14020401	31354 [†]	20
Caelo	Viscous base solution (NRF p...	14109401	31658 [†]	20
Caelo	Viscous base solution (NRF p...	15265401	31790 [†]	20
Caelo	Viscous base solution (NRF p...	153888	31882	60
Caelo	Viscous base solution (NRF p...	153888	31883	60
Caelo	Viscous base solution (NRF p...	153888	31884 [†]	20
Caelo	Viscous base solution (NRF p...	153889	31885	60
Caelo	Viscous base solution (NRF p...	153889	31886 [†]	20
Caelo	Viscous base solution (NRF p...	154121	31887 [†]	20
Caelo	Viscous base solution (NRF p...	154121	31888	60

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

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Viscous base solution (NRF p...	153890	31889	60
Caelo	Viscous base solution (NRF p...	153890	31890 [†]	20
Caelo	Viscous base solution (NRF p...	153892	31891	60
Caelo	Viscous base solution (NRF p...	153893	31892	60
Caelo	Viscous base solution (NRF p...	153894	31893 [†]	20
Caelo	Viscous base solution (NRF p...	153894	31894	60
Caelo	Viscous base solution (NRF p...	153895	31895	60
Caelo	Viscous base solution (NRF p...	153895	31896 [†]	20
Caelo	Viscous base solution (NRF p...	153896	31897 [†]	20
Caelo	Viscous base solution (NRF p...	153896	31898	60
Caelo	Viscous base solution (NRF p...	153897	31899	60
Caelo	Viscous base solution (NRF p...	153897	31900 [†]	20
Caelo	Viscous base solution (NRF p...	161076	32287	40
Caelo	Viscous base solution (NRF p...	161089	32288	40
Caelo	Viscous base solution (NRF p...	161090	32289	40
Caelo	Viscous base solution (NRF p...	162172	32356	40
Caelo	Viscous base solution (NRF p...	162173	32357	40
Caelo	Viscous base solution (NRF p...	162174	32358	40
Caelo	Viscous base solution (NRF p...	162175	32359	40
Caelo	Viscous base solution (NRF p...	162176	32360	40
Caelo	Viscous base solution (NRF p...	162297	32554	40
Caelo	Viscous base solution (NRF p...	162298	32555	40
Caelo	Viscous base solution (NRF p...	162299	32556	40
Caelo	Viscous base solution (NRF p...	162300	32557	40
Caelo	Viscous base solution (NRF p...	162301	32558	40
Caelo	Viscous base solution (NRF p...	162650	32559	40
Caelo	Viscous base solution (NRF p...	162651	32572	40
Caelo	Viscous base solution (NRF p...	162652	32573	40
Caelo	Viscous base solution (NRF p...	162653	32574	40
Caelo	Viscous base solution (NRF p...	162655	32575	40
Caelo	Viscous base solution (NRF p...	163153	32897	40
Caelo	Viscous base solution (NRF p...	163152	32898	40

- 61 834 spectra from a total of 1442 batches from further 439 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.

- 665 spectra from 52 *Apo-Ident* customers from 282 batches from the substance/substance group *Viscous base solution (NRF p.20.)*.

Supplier	Substance	Batch	Spectra
Fagron	Viscous base solution (NRF p...	1301F003	3
Apomix / 11ol	Viscous base solution (NRF p...	13229501	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	11214	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
Sonnenberg Apotheke	Viscous base solution (NRF p...	30216	1
Caelo	Viscous base solution (NRF p...	1071501	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	20516	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	10814	1
Caelo	Viscous base solution (NRF p...	5051502	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	2012015	2
Sonnenberg-Apotheke	Viscous base solution (NRF p...	40117	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	70514	1
Sonnenberg Apotheke	Viscous base solution (NRF p...	71015	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	70916	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	90714	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	71216	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	100314	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	90414	1
Sonnenberg Apotheke	Viscous base solution (NRF p...	90915	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	91116	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	100715	1
Fagron	Viscous base solution (NRF p...	10031502	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	100914	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	110116	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	111114	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	110516	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	110614	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	111115	1
Fagron	Viscous base solution (NRF p...	1301F001	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	121016	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	130416	1
Fagron	Viscous base solution (NRF p...	1310167	9
Aliance am 08.04.2014	Viscous base solution (NRF p...	1306F002	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	131014	1
Fagron	Viscous base solution (NRF p...	13J22-T05-007720	1
Caelo	Viscous base solution (NRF p...	13229502	3
Fagron	Viscous base solution (NRF p...	1310F006	1
Caelo	Viscous base solution (NRF p...	13157701	1
Caelo	Viscous base solution (NRF p...	14000901	2
Fagron	Viscous base solution (NRF p...	13J22-T05-007729	8
Caelo	Viscous base solution (NRF p...	14000801	6
Caelo	Viscous base solution (NRF p...	14020301	5
Caelo	Viscous base solution (NRF p...	14020401	9
Caelo	Viscous base solution (NRF p...	14020402	3
Gutenberg-Apotheke	Viscous base solution (NRF p...	14020502	1
Fagron	Viscous base solution (NRF p...	14020502	5
GEHE am 27.05.2014	Viscous base solution (NRF p...	14020502	1
Fagron	Viscous base solution (NRF p...	1402F001	25
Caelo	Viscous base solution (NRF p...	14020701	1
Caelo	Viscous base solution (NRF p...	14058901	3
Caelo	Viscous base solution (NRF p...	14059001	2
Fagron	Viscous base solution (NRF p...	14059001	2
Gutenberg-Apotheke	Viscous base solution (NRF p...	14059101	3
Caelo	Viscous base solution (NRF p...	14059101	5
Caelo	Viscous base solution (NRF p...	14109401	4
Caelo	Viscous base solution (NRF p...	14059301	1
Caelo	Viscous base solution (NRF p...	14109402	3
Sanacorp	Viscous base solution (NRF p...	14109402	1
Caelo	Viscous base solution (NRF p...	14109501	5
Caelo	Viscous base solution (NRF p...	14109801	3
Caelo	Viscous base solution (NRF p...	14109701	1
Caelo	Viscous base solution (NRF p...	14109901	11
Alliance Health.18.09.2...	Viscous base solution (NRF p...	14109901	1
Phoenix 08.07.2014	Viscous base solution (NRF p...	14110001	1

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Supplier	Substance	Batch	Spectra
Caelo	Viscous base solution (NRF p...	14110001	2
Caelo	Viscous base solution (NRF p...	14187201	9
Caelo	Viscous base solution (NRF p...	1418730	2
Caelo	Viscous base solution (NRF p...	14187301	7
Caelo	Viscous base solution (NRF p...	14187601	5
Caelo	Viscous base solution (NRF p...	14187501	1
Gehe 19.12.14	Viscous base solution (NRF p...	14187601	1
Caelo	Viscous base solution (NRF p...	14187801	11
Caelo	Viscous base solution (NRF p...	14187701	1
Caelo	Viscous base solution (NRF p...	14187901	2
Caelo	Viscous base solution (NRF p...	14188001	5
Caelo	Viscous base solution (NRF p...	14266501	7
Caelo	Viscous base solution (NRF p...	14266101	1
Caelo	Viscous base solution (NRF p...	14266601	2
Caelo	Viscous base solution (NRF p...	14354304	3
Caelo	Viscous base solution (NRF p...	14354401	2
Caelo	Viscous base solution (NRF p...	14354501	1
Caelo	Viscous base solution (NRF p...	14368401	4
Caelo	Viscous base solution (NRF p...	14368601	8
Caelo	Viscous base solution (NRF p...	14368701	3
Sonnenberg Apotheke	Viscous base solution (NRF p...	150616	1
Caelo	Viscous base solution (NRF p...	15093301	8
Caelo	Viscous base solution (NRF p...	14368801	1
Caelo	Viscous base solution (NRF p...	15093401	4
Caelo	Viscous base solution (NRF p...	15093501	2
Caelo	Viscous base solution (NRF p...	15093601	1
Caelo	Viscous base solution (NRF p...	15093602	3
Caelo	Viscous base solution (NRF p...	15093701	3
Caelo	Viscous base solution (NRF p...	15093801	1
Caelo	Viscous base solution (NRF p...	15105701	4
Caelo	Viscous base solution (NRF p...	15141601	2
Caelo	Viscous base solution (NRF p...	15141901	2
Caelo	Viscous base solution (NRF p...	15196701	1
Caelo	Viscous base solution (NRF p...	15180101	1
Caelo	Viscous base solution (NRF p...	152364901	1
Caelo	Viscous base solution (NRF p...	15196601	1
Caelo	Viscous base solution (NRF p...	15264801	7
Caelo	Viscous base solution (NRF p...	15264901	1
Caelo	Viscous base solution (NRF p...	15265201	3
Caelo	Viscous base solution (NRF p...	15265101	1
Caelo	Viscous base solution (NRF p...	15265001	1
Caelo	Viscous base solution (NRF p...	15265301	6
Sanacorp	Viscous base solution (NRF p...	15265201	1
Caelo	Viscous base solution (NRF p...	15265501	5
Caelo	Viscous base solution (NRF p...	15265402	1
Caelo	Viscous base solution (NRF p...	15265601	2
Caelo	Viscous base solution (NRF p...	15265701	4
Caesar&Loretz GmbH	Viscous base solution (NRF p...	15265701	1
Caelo	Viscous base solution (NRF p...	15265801	2
Caelo	Viscous base solution (NRF p...	15265901	3
Caelo	Viscous base solution (NRF p...	15389401	3
Caelo	Viscous base solution (NRF p...	15389501	1
Caelo	Viscous base solution (NRF p...	15389701	6
Sonnenberg-Apotheke	Viscous base solution (NRF p...	160415	1
Caelo	Viscous base solution (NRF p...	15412101	2
Sonnenberg-Apotheke	Viscous base solution (NRF p...	160316	1
Defektur Bahnhof Apotheke	Viscous base solution (NRF p...	160630008	1
Defektur Bahnhof Apotheke	Viscous base solution (NRF p...	160630007	1
Defektur Bahnhof Apotheke	Viscous base solution (NRF p...	160805001	1
Defektur Bahnhof Apotheke	Viscous base solution (NRF p...	160719002	1

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Supplier	Substance	Batch	Spectra
Bahnhof Apotheke	Viscous base solution (NRF p...	160818002	1
Defektur Bahnhof Apotheke	Viscous base solution (NRF p...	160805002	1
Defektur Bahnhof Apotheke	Viscous base solution (NRF p...	160718007	1
Bahnhof Apotheke	Viscous base solution (NRF p...	160818001	1
Bahnhof-Apotheke	Viscous base solution (NRF p...	160823001	1
Bahnhof-Apotheke	Viscous base solution (NRF p...	160825001	1
Bahnhof-Apotheke	Viscous base solution (NRF p...	160825002	1
Caelo	Viscous base solution (NRF p...	16107601	1
Caesar&Loretz GmbH	Viscous base solution (NRF p...	16107601	3
Caelo	Viscous base solution (NRF p...	16108101	1
Caelo	Viscous base solution (NRF p...	16108001	2
Caelo	Viscous base solution (NRF p...	16108301	2
Caelo	Viscous base solution (NRF p...	16108501	3
Caelo	Viscous base solution (NRF p...	16108401	1
Caelo	Viscous base solution (NRF p...	16108901	3
Caesar&Loretz GmbH	Viscous base solution (NRF p...	16108901	1
Caelo	Viscous base solution (NRF p...	16108601	2
Jenne	Viscous base solution (NRF p...	16108901	1
Caelo	Viscous base solution (NRF p...	16109001	1
Caelo	Viscous base solution (NRF p...	16315201	2
Sonnenberg-Apotheke	Viscous base solution (NRF p...	161215	1
Caesar&Loretz GmbH	Viscous base solution (NRF p...	16217301	1
Caesar&Loretz GmbH	Viscous base solution (NRF p...	16229701	1
Caelo	Viscous base solution (NRF p...	18071502	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	211216	1
Caelo	Viscous base solution (NRF p...	20081501	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	220216	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	231116	1
Sonnenberg Apotheke	Viscous base solution (NRF p...	220616	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	230315	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	250215	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	250716	1
Fagron	Viscous base solution (NRF p...	28111402	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	280916	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	261016	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	260115	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	290716	1
Sonnenberg Apotheke	Viscous base solution (NRF p...	270515	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	290716-2	1
Sonnenberg Apotheke	Viscous base solution (NRF p...	300615	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	60114	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	91213	1
Sonnenberg-Apotheke	Viscous base solution (NRF p...	100214	1
Caelo	Viscous base solution (NRF p...	3x14058901	1
Fagron	Viscous base solution (NRF p...	1111F001	1
Fagron	Viscous base solution (NRF p...	1111F003	1
Klenk	Viscous base solution (NRF p...	1111F003	1
Caelo	Viscous base solution (NRF p...	11140501	1
Noweda	Viscous base solution (NRF p...	11176201	1
Caelo	Viscous base solution (NRF p...	11176401	1
Caelo	Viscous base solution (NRF p...	12019001	1
Anzag	Viscous base solution (NRF p...	12018901	1
Caelo	Viscous base solution (NRF p...	12019002	2
Gehe	Viscous base solution (NRF p...	12019201	1
Fagron	Viscous base solution (NRF p...	1203C004	2
Noweda	Viscous base solution (NRF p...	12019401	1
Fagron	Viscous base solution (NRF p...	1206F003	3
Caelo	Viscous base solution (NRF p...	12094101	2
Noweda	Viscous base solution (NRF p...	12093601	2
Anzag 05.09.2012	Viscous base solution (NRF p...	12127302	4

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Supplier	Substance	Batch	Spectra
Caelo	Viscous base solution (NRF p...	12093801	1
Caelo	Viscous base solution (NRF p...	12093901	1
Caelo	Viscous base solution (NRF p...	12093701	1
Sanacorp	Viscous base solution (NRF p...	12127401	2
Caelo	Viscous base solution (NRF p...	12127601	2
Phönix 11.03.2013	Viscous base solution (NRF p...	12127601	2
Fagron	Viscous base solution (NRF p...	1214509	1
Caelo	Viscous base solution (NRF p...	12231002	1
Caelo	Viscous base solution (NRF p...	12231101	5
Caelo	Viscous base solution (NRF p...	12231201	1
Caelo	Viscous base solution (NRF p...	12249801	1
Sanacorp	Viscous base solution (NRF p...	12231301	4
Caelo	Viscous base solution (NRF p...	12249901	3
Caelo	Viscous base solution (NRF p...	1224991	1
Gehe am 28.01.2013	Viscous base solution (NRF p...	12250101	3
Caelo	Viscous base solution (NRF p...	12309001	2
Caelo	Viscous base solution (NRF p...	12309101	11
Caelo	Viscous base solution (NRF p...	12309201	6
Phoenix 11.03.2013	Viscous base solution (NRF p...	12309202	5
Apomix / 11	Viscous base solution (NRF p...	12309201	1
Phönix 04.04.13	Viscous base solution (NRF p...	13006001	6
Caelo	Viscous base solution (NRF p...	12309202	1
Caelo	Viscous base solution (NRF p...	13006001	1
Caelo	Viscous base solution (NRF p...	13006201	4
Caelo	Viscous base solution (NRF p...	13006301	5
Caelo	Viscous base solution (NRF p...	13006401	6
Caelo	Viscous base solution (NRF p...	13006501	2
Fagron	Viscous base solution (NRF p...	1301673	4
Phönix 11.11.2014	Viscous base solution (NRF p...	1301F001	1
Fagron	Viscous base solution (NRF p...	1301F002	3
Fagron	Viscous base solution (NRF p...	1302F002	18
Post Apotheke	Viscous base solution (NRF p...	1306F002	2
Caelo	Viscous base solution (NRF p...	13096001	2
Caelo	Viscous base solution (NRF p...	13071302	1
Caelo	Viscous base solution (NRF p...	13096101	6
Herstellung	Viscous base solution (NRF p...	131030004	1
Herstellung	Viscous base solution (NRF p...	131018001	1
Herstellung	Viscous base solution (NRF p...	131025001	1
Herstellung	Viscous base solution (NRF p...	131030005	1
Herstellung	Viscous base solution (NRF p...	131018004	1
Herstellung	Viscous base solution (NRF p...	131115001	1
Herstellung	Viscous base solution (NRF p...	131126002	2
Herstellung	Viscous base solution (NRF p...	131211001	1
Herstellung	Viscous base solution (NRF p...	131211002	1
Herstellung	Viscous base solution (NRF p...	131203012	1
Herstellung	Viscous base solution (NRF p...	131206001	1
Herstellung	Viscous base solution (NRF p...	131218006	1
Herstellung	Viscous base solution (NRF p...	131220001	1
Post-Apotheke	Viscous base solution (NRF p...	13150801	3
Caelo	Viscous base solution (NRF p...	13150801	3
Caelo	Viscous base solution (NRF p...	13150802	2
Caelo	Viscous base solution (NRF p...	13151101	6
Caelo	Viscous base solution (NRF p...	13151201	4
Caelo	Viscous base solution (NRF p...	13158001	9
Caelo	Viscous base solution (NRF p...	13158002	1
Caelo	Viscous base solution (NRF p...	1315801	1
Caesar & Loretz GmbH	Viscous base solution (NRF p...	13158201	1
Phönix 11.11.2013	Viscous base solution (NRF p...	13158101	1
Caelo	Viscous base solution (NRF p...	13158201	2
Caelo	Viscous base solution (NRF p...	13228901	8

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Supplier	Substance	Batch	Spectra
Caelo	Viscous base solution (NRF p...	13220101	1
Caelo	Viscous base solution (NRF p...	13229001	3
Caelo	Viscous base solution (NRF p...	13229201	1
Caelo	Viscous base solution (NRF p...	13229501	4
Caelo	Viscous base solution (NRF p...	13229101	1
Alliance Health 21.02.2...	Viscous base solution (NRF p...	13229502	2
Caelo	Viscous base solution (NRF p...	13246101	1
Caelo	Viscous base solution (NRF p...	13246401	5
Caelo	Viscous base solution (NRF p...	13246501	5
Caelo	Viscous base solution (NRF p...	13246901	1
Caelo	Viscous base solution (NRF p...	13246701	3
Herstellung	Viscous base solution (NRF p...	140108003	1
Herstellung	Viscous base solution (NRF p...	140108002	1
Herstellung	Viscous base solution (NRF p...	140117001	1
Caelo	Viscous base solution (NRF p...	14020601	3
Bombastus	Viscous base solution (NRF p...	15265501	1
Herstellung	Viscous base solution (NRF p...	20010213-1	1
Herstellung	Viscous base solution (NRF p...	20030513-1	1
Herstellung	Viscous base solution (NRF p...	20041013-1	1
Herstellung	Viscous base solution (NRF p...	20040113-1	1
Herstellung	Viscous base solution (NRF p...	20040113-2	1
Herstellung	Viscous base solution (NRF p...	20050613-1	1
Herstellung	Viscous base solution (NRF p...	20050713-1	1
Herstellung	Viscous base solution (NRF p...	20050713-2	1
Herstellung	Viscous base solution (NRF p...	20060913-2	1
Herstellung	Viscous base solution (NRF p...	20090113-1	2
Herstellung	Viscous base solution (NRF p...	20060913-1	1
Herstellung	Viscous base solution (NRF p...	20080313-1	1
Herstellung	Viscous base solution (NRF p...	20080213-1	1
Herstellung	Viscous base solution (NRF p...	20100513-1	1
Herstellung	Viscous base solution (NRF p...	20130313-1	1
Herstellung	Viscous base solution (NRF p...	20100613-1	1
Herstellung	Viscous base solution (NRF p...	20130613-1	1
Herstellung	Viscous base solution (NRF p...	20140613-1	1
Herstellung	Viscous base solution (NRF p...	20120713-1	1
Herstellung	Viscous base solution (NRF p...	20150813-3	1
Herstellung	Viscous base solution (NRF p...	20150213-1	1
Herstellung	Viscous base solution (NRF p...	20150813-4	1
Herstellung	Viscous base solution (NRF p...	20160513-2	1
Herstellung	Viscous base solution (NRF p...	20190413-1	1
Herstellung	Viscous base solution (NRF p...	20210313-1	1
Herstellung	Viscous base solution (NRF p...	20190413-2	1
Herstellung	Viscous base solution (NRF p...	20200913-1	1
Herstellung	Viscous base solution (NRF p...	20220213-1	1
Herstellung	Viscous base solution (NRF p...	20210313-2	1
Caelo	Viscous base solution (NRF p...	20250113-1	1
Herstellung	Viscous base solution (NRF p...	20220213-2	1
Herstellung	Viscous base solution (NRF p...	20220513-2	1
Herstellung	Viscous base solution (NRF p...	20260313-2	1
Herstellung	Viscous base solution (NRF p...	20260713-1	1
Herstellung	Viscous base solution (NRF p...	20260313-1	1
Herstellung	Viscous base solution (NRF p...	20260713-2	1
Herstellung	Viscous base solution (NRF p...	20270913-2	1
Herstellung	Viscous base solution (NRF p...	20280513-1	1
Herstellung	Viscous base solution (NRF p...	20280613-2	1
Herstellung	Viscous base solution (NRF p...	20280613-1	1
Herstellung	Viscous base solution (NRF p...	2030913-1	1
Herstellung	Viscous base solution (NRF p...	20300713-2	1
Herstellung	Viscous base solution (NRF p...	2150313-1	1
Fagron	Viscous base solution (NRF p...	22041304	2

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Supplier	Substance	Batch	Spectra
Caelo	Viscous base solution (NRF p...	3013A-03142	1
Fagron	Viscous base solution (NRF p...	31101205	1
Anzag, 18.07.2012	Viscous base solution (NRF p...		1
Herstellung	Viscous base solution (NRF p...	240114	1

- 57 776 spectra from 332 *Apo-Ident* customers from a total of 19 815 batches from a further 328 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 *Viscous base solution (NRF p.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 *Viscous base solution (NRF p.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	480	0	33 864
Type B	0	1750	10	61 834
Type C	0	643	22	57 776

The substance/substance group *Viscous base solution (NRF p.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 % (> 99.9689 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9710 %)	99.4318 % (> 99.2614 %)
Type C	100.0000 % (> 99.5963 %)	96.6917 % (> 96.2406 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30659	30659	0.00	26.49
31354	31900	1.53	23.89
31658	31658	0.00	28.05
31790	31893	3.88	28.08
31884	31884	0.00	28.03
31886	31886	0.00	27.80
31887	31887	0.00	27.68
31890	31890	0.00	27.73
31893	31893	0.00	27.67
31896	31896	0.00	27.57
31897	31897	0.00	27.23
31900	31900	0.00	28.31

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Water and aqueous solutions
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30869-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Water and aqueous solutions; Aluminium acetate tartrate solution; Aqua; Chlorhexidine digluconate solution 20%; Chlorhexidini digluconatis solutio 20%; Liquor aluminii acetico-tartarici; Solutio chlorhexidini gluconici 20%; 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

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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	Aluminium acetat...	12233502	30869	40	20120810
Caelo	Water	13176101	31057	40	20130627
Fagron	Chlorhexidine di...	13H19-B01	31240	30	20130906

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Aluminium acetat. ...	13378704	31342	40	AR-14-FG-012698-01
Caelo	Chlorhexidine di. ...	14011009	31463	40	AR-15-FG-010164-03
Caelo	Water	14253301	31624	40	20140923
Fagron	Water	14K05-T02-016775	31676	40	20150225
Caelo	Chlorhexidine di. ...	15131504	31705	40	20150424
Caelo	Water	15142501	31718	40	1510212
Euro OTC	Chlorhexidine di. ...	1508022	31735	40	20150916*
Fagron	Water	15D01-C20-16500	31809	40	20151105
Fagron	Chlorhexidine di. ...	15I03-B02-315213	31829	30	20151027
Euro OTC	Chlorhexidine di. ...	1511039	31846	40	20160114*
Caelo	Aluminium acetat. ...	15299901	31959	40	20151001
Caelo	Chlorhexidine di. ...	15292508	32308	40	20151109
Caelo	Water	161975	32354	30	20160725*
Euro OTC	Chlorhexidine di. ...	1511033-01	32732	40	20160114
Euro OTC	Chlorhexidine di. ...	1610021	32831	40	20161121*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 690 spectra of 18 reference samples from the substance/substance group *Water and aqueous solutions*. These samples are listed above in the [calibration samples](#) section.
- 33 654 spectra from a total of 780 batches from further 222 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 695 spectra of 23 reference samples from the substance/substance group *Water and aqueous solutions*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Chlorhexidine digluconate so. ...	82369169	30005	20
Fagron	Chlorhexidine digluconate so. ...	11C16-N07	30246	40
Fagron	Chlorhexidine digluconate so. ...	10H24-N08	30268	40
Caelo	Chlorhexidine digluconate so. ...	14011009	31463 [†]	20

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

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Water	14253301	31624 [†]	20
Fagron	Water	14K05-T02-016775	31676 [†]	20
Caelo	Chlorhexidine digluconate so...	15131504	31705 [†]	20
Caelo	Water	15142501	31718 [†]	20
Euro OTC	Chlorhexidine digluconate so...	1508022	31735 [†]	20
Fagron	Water	15D01-C20-16500	31809 [†]	20
Fagron	Chlorhexidine digluconate so...	15I03-B02-315213	31829 [†]	15
Euro OTC	Chlorhexidine digluconate so...	1511039	31846 [†]	20
Caelo	Aluminium acetate tartrate s...	1529901	31959 [†]	20
Caelo	Water	153714	32080	40
Caelo	Water	153945	32082	40
Caelo	Water	162119	32353	40
Caelo	Water	162230	32355	40
Euro OTC	Chlorhexidine digluconate so...	1610022	32832	40
Caelo	Water	163133	32893	40
Caelo	Water	162554	32894	40
Hedinger	Aluminium acetate tartrate s...	20160B	32921	40
Fagron	Water	16K25-C20-17409	32963	40
Caelo	Chlorhexidine digluconate so...	163088	33089	40

- 62 899 spectra from a total of 1454 batches from further 437 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.

- 1389 spectra from 243 *Apo-Ident* customers from 418 batches from the substance/substance group *Water and aqueous solutions*.

Supplier	Substance	Batch	Spectra
Franz GmbH	Aluminium acetate tartrate s...	20152B	2
Hedinger/Gehe	Aluminium acetate tartrate s...	20153B	2
Hedinger	Aluminium acetate tartrate s...	20154B	11
Hedinger/Noweda	Aluminium acetate tartrate s...	200161B	1
Gehe	Aluminium acetate tartrate s...	20155B	1
Hedinger	Aluminium acetate tartrate s...	20155B	9
Phönix/Hedinger	Aluminium acetate tartrate s...	20155B	3
Caelo	Aluminium acetate tartrate s...	20155B	4
Franz GmbH	Aluminium acetate tartrate s...	20155B	3
Sanacorp	Aluminium acetate tartrate s...	20155B	1
Hedinger/Noweda	Aluminium acetate tartrate s...	20155B	1
Hedinger / Sanacorp	Aluminium acetate tartrate s...	20155B	1
Hedinger über Phoenix	Aluminium acetate tartrate s...	20155B	1
Hedinger / Alliance Hea...	Aluminium acetate tartrate s...	20155B	1
Caelo	Aluminium acetate tartrate s...	201563	1
Raben-Apotheke Mildenau	Aluminium acetate tartrate s...	20156B	5

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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
Gehe Kassel	Aluminium acetate tartrate s...	201568B	1
Hedinger	Aluminium acetate tartrate s...	20156B	11
Hedinger/Noweda	Aluminium acetate tartrate s...	201568	1
Caelo	Aluminium acetate tartrate s...	20156B	3
Hedinger / Gehe	Aluminium acetate tartrate s...	20156B	2
Hedinger/Jenne 16.08.14	Aluminium acetate tartrate s...	20156B	1
Hedinger / Sanacorp	Aluminium acetate tartrate s...	20156B	1
Hedinger/Noweda	Aluminium acetate tartrate s...	20156B	3
Hediger/Phönix	Aluminium acetate tartrate s...	20156B	1
hedinger/Gehe	Aluminium acetate tartrate s...	20156B	1
Hedinger/Phönix	Aluminium acetate tartrate s...	20156B	1
Hedinger/Phoenix	Aluminium acetate tartrate s...	201578	1
Noweda/Hedinger	Aluminium acetate tartrate s...	20156B	1
Hedinger	Aluminium acetate tartrate s...	20157B	6
Hedinger / Gehe	Aluminium acetate tartrate s...	20157B	1
hedinger	Aluminium acetate tartrate s...	20157B	1
hedinger/phönix	Aluminium acetate tartrate s...	20157B	1
GEHE 08.05	Aluminium acetate tartrate s...	20157B	1
Hedinger über Phoenix	Aluminium acetate tartrate s...	20157B	1
Hedinger/Gehe	Aluminium acetate tartrate s...	20157B	1
Hedinger/Phoenix	Aluminium acetate tartrate s...	20158B	1
Spangro/Hedinger	Aluminium acetate tartrate s...	20158B	1
Hedinger/Noweda	Aluminium acetate tartrate s...	20158B	1
hedinger	Aluminium acetate tartrate s...	201598	1
Hedinger	Aluminium acetate tartrate s...	20158B	2
Hedinger / Noweda	Aluminium acetate tartrate s...	201598	1
Hedinger/ Phönix	Aluminium acetate tartrate s...	20159B	1
Hedinger/Phönix	Aluminium acetate tartrate s...	20159B	3
Caelo	Aluminium acetate tartrate s...	20159B	2
HEDINGER/NOWEDA	Aluminium acetate tartrate s...	20159B	1
Hedinger/Phoenix	Aluminium acetate tartrate s...	20159B	3
Hedinger/Alliance Healt...	Aluminium acetate tartrate s...	20159B	1
Hedinger/Sana	Aluminium acetate tartrate s...	20159B	1
Kehr/gepepharm	Aluminium acetate tartrate s...	20160B	1
Hedinger	Aluminium acetate tartrate s...	20160B	2
Aug. Hedinger GmbH & Co...	Aluminium acetate tartrate s...	20161B	1
Hedinger/Phoenix	Aluminium acetate tartrate s...	20160B	2
Haedinger	Aluminium acetate tartrate s...	20160B	1
Hedinger	Aluminium acetate tartrate s...	5081403	1
Hedinger	Aluminium acetate tartrate s...	20161B	3
Gehe	Aluminium acetate tartrate s...	20160B	2
Hedinger / Noweda	Aluminium acetate tartrate s...	20161B	1
Jenne	Aluminium acetate tartrate s...	20161B	1
Caelo	Aluminium acetate tartrate s...	6031415	1
athenstaedt GmbH / Noweda	Aluminium acetate tartrate s...	110024	1
athenstaedt	Aluminium acetate tartrate s...	110024	1
Caelo	Aluminium acetate tartrate s...	12318703	1
Caelo	Aluminium acetate tartrate s...	13261302	1
Caelo	Aluminium acetate tartrate s...	13261303	1
Caelo	Aluminium acetate tartrate s...	13378701	2
Caelo	Aluminium acetate tartrate s...	13261304	3
Phönix Gotha	Aluminium acetate tartrate s...	13261304	1
Euro OTC	Aluminium acetate tartrate s...	13378701	1
Caelo	Aluminium acetate tartrate s...	13378703	1
Caelo	Aluminium acetate tartrate s...	13378709	2
Caelo	Aluminium acetate tartrate s...	13378708	2
Caelo	Aluminium acetate tartrate s...	14071503	1
Caelo	Aluminium acetate tartrate s...	1425006	1
Caelo	Aluminium acetate tartrate s...	14252009	1
Caelo	Aluminium acetate tartrate s...	13378704	1

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Supplier	Substance	Batch	Spectra
Caelo	Aluminium acetate tartrate s...	1425010	1
Caelo	Aluminium acetate tartrate s...	14252010	2
Caesar&Loretz GmbH/Anzag	Aluminium acetate tartrate s...	14252010	1
Fagron	Aluminium acetate tartrate s...	14252010	1
Caelo	Aluminium acetate tartrate s...	1504506	1
Caelo	Aluminium acetate tartrate s...	15045405	4
Caelo	Aluminium acetate tartrate s...	15045403	3
Caelo	Aluminium acetate tartrate s...	15045406	5
Caelo	Aluminium acetate tartrate s...	15299901	3
Caelo	Aluminium acetate tartrate s...	15299902	2
Caelo	Aluminium acetate tartrate s...	15299909	2
Bombastus	Aluminium acetate tartrate s...	160029	1
Cealo/AHD	Aluminium acetate tartrate s...	15299909	1
Hedinger/Phönix	Aluminium acetate tartrate s...	(020)020	1
Hedinger	Aluminium acetate tartrate s...	20149B	1
Hedinger, Heiligenwiese...	Aluminium acetate tartrate s...	20150B	1
Kehr	Aluminium acetate tartrate s...	20150B	1
Hedinger/ Noweda	Aluminium acetate tartrate s...	20149B	1
Caelo	Aluminium acetate tartrate s...	20150B	2
Sanacorp	Aluminium acetate tartrate s...	20150B	1
Hedinger	Aluminium acetate tartrate s...	20150B	4
Noweda	Aluminium acetate tartrate s...	20150B	1
Hedinger	Aluminium acetate tartrate s...	20150b	1
Hedinger	Aluminium acetate tartrate s...	20151B	8
Kehr	Aluminium acetate tartrate s...	20151B	1
Stumpf	Aluminium acetate tartrate s...	20151B	1
Hedinger	Aluminium acetate tartrate s...	20150B	1
Hedinger	Aluminium acetate tartrate s...	20151B	1
Anzag/	Aluminium acetate tartrate s...	20151B	1
hedinger	Aluminium acetate tartrate s...	20151B	1
Noweda	Aluminium acetate tartrate s...	20151B	1
Großhandel	Aluminium acetate tartrate s...	20151B	1
Caelo	Aluminium acetate tartrate s...	20151B	1
Hedinger/Noweda	Aluminium acetate tartrate s...	20151B	1
Franz GmbH/Phönix	Aluminium acetate tartrate s...	20151B	1
Hedinger/Phönix	Aluminium acetate tartrate s...	20152B	2
Dr.Seeger GmbH	Aluminium acetate tartrate s...		1
PHÖNIX 05.06.2013	Aluminium acetate tartrate s...	20151B	1
hedinger	Aluminium acetate tartrate s...	201528	1
Anzag	Aluminium acetate tartrate s...	20152B	2
Hedinger	Aluminium acetate tartrate s...	20152B	6
Caelo	Aluminium acetate tartrate s...	20152b	1
Hedinger / Gehe	Aluminium acetate tartrate s...	20152B	1
Caelo	Aluminium acetate tartrate s...	20152B	2
Fischar/Anzag	Aluminium acetate tartrate s...	20152B	1
Anzag 17.04.13 ek: 5,43EUR	Aluminium acetate tartrate s...	20152B	1
Hedinger/Gehe	Aluminium acetate tartrate s...	20152B	1
Hedinger/Otto	Aluminium acetate tartrate s...	201538	1
Franz/Noweda	Aluminium acetate tartrate s...	201538	3
franz gmbh	Aluminium acetate tartrate s...	201538	1
Caelo	Aluminium acetate tartrate s...	201538	2
Hedinger	Aluminium acetate tartrate s...	201538	2
Spangr/Hedinger	Aluminium acetate tartrate s...	201538	1
Hedinger	Aluminium acetate tartrate s...	20153B	8
Hedinger , Noweda	Aluminium acetate tartrate s...	20153B	1
Gehe/Hedinger	Aluminium acetate tartrate s...	20153B	1
Gehe	Aluminium acetate tartrate s...	20153B	1
Hedinger/Sanacorp	Aluminium acetate tartrate s...	20153B	2
Hedinger/Phönix	Aluminium acetate tartrate s...	20153B	2
Dr. Seeger	Aluminium acetate tartrate s...	20153B	1

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Supplier	Substance	Batch	Spectra
hedinger/anzag	Aluminium acetate tartrate s...	20153b	1
Phönix	Aluminium acetate tartrate s...	20153b	1
Caelo	Aluminium acetate tartrate s...	20153B	2
Dr.Seeger GmbH	Aluminium acetate tartrate s...	20153B	1
Noweda/Hedinger	Aluminium acetate tartrate s...	20153B	1
geile	Aluminium acetate tartrate s...	20154B	1
Hedinger	Aluminium acetate tartrate s...	201548	1
Caelo	Aluminium acetate tartrate s...	20154B	5
Hedinger/V.d.L.	Aluminium acetate tartrate s...	20154B	1
Hedinger/ Sanacorp	Aluminium acetate tartrate s...	20154B	1
hedinger/gehe	Aluminium acetate tartrate s...	20154B	1
Hedinger, Noweda	Aluminium acetate tartrate s...	20154B	2
Hedinger , Stuttgart	Aluminium acetate tartrate s...	20154B	1
Hedinger/Sanacorp	Aluminium acetate tartrate s...	20154B	1
hedinger/Gehe	Aluminium acetate tartrate s...	20155B	1
hedinger/phönix	Aluminium acetate tartrate s...	20155B	1
Hedinger/GEHE	Aluminium acetate tartrate s...	20155B	1
Hedinger	Aluminium acetate tartrate s...	2153B	1
Hedinger	Aluminium acetate tartrate s...	402211793	1
Athenstaedt	Aluminium acetate tartrate s...	900108	2
heidinger/noweda	Aluminium acetate tartrate s...	20156B	1
athenstaedt GmbH	Aluminium acetate tartrate s...	900107	2
Phönix Gotha	Aluminium acetate tartrate s...	900108	2
athenstedt	Aluminium acetate tartrate s...	110029	1
Hedinger	Aluminium acetate tartrate s...	2021302	1
Hedinger/Phönix	Aluminium acetate tartrate s...	2015B	1
Hedinger	Aluminium acetate tartrate s...	2015B	1
Caelo	Aluminium acetate tartrate s...	11315007	1
Hedinger	Aluminium acetate tartrate s...	1111	1
Caelo	Aluminium acetate tartrate s...	11315004	1
Caelo	Aluminium acetate tartrate s...	11315002	1
Caesar&lorenz,Phoenix	Aluminium acetate tartrate s...	12116804	1
Caelo	Aluminium acetate tartrate s...	12116804	5
Caelo	Aluminium acetate tartrate s...	12116803	3
Caelo	Aluminium acetate tartrate s...	12233501	4
Caelo	Aluminium acetate tartrate s...	12233502	4
Caelo	Aluminium acetate tartrate s...	12233503	1
Caelo	Aluminium acetate tartrate s...	12233504	1
Caelo	Aluminium acetate tartrate s...	12318701	6
Phönix	Aluminium acetate tartrate s...	12318705	1
Caelo	Aluminium acetate tartrate s...	12318704	2
Phönix	Aluminium acetate tartrate s...	12318703	1
Caelo	Aluminium acetate tartrate s...	12318702	1
Caelo	Aluminium acetate tartrate s...	12318705	2
Caelo	Aluminium acetate tartrate s...	13101101	1
Caelo	Aluminium acetate tartrate s...	13101102	5
Phönix	Aluminium acetate tartrate s...	13101101	1
Caelo	Aluminium acetate tartrate s...	13101104	5
Caelo	Aluminium acetate tartrate s...	13261301	3
Calo/AHD	Aluminium acetate tartrate s...	13101105	1
Caelo	Aluminium acetate tartrate s...	13261306	1
Hedinger Phönix	Aluminium acetate tartrate s...	201528	1
Caesar&Loretz GmbH/Anzag	Aluminium acetate tartrate s...	13101105	1
Caelo	Aluminium acetate tartrate s...	13261307	1
Hedinger	Aluminium acetate tartrate s...	26041301	1
Caelo	Aluminium acetate tartrate s...	17081201	1
Caelo	Aluminium acetate tartrate s...	2713M-01793	1
Hedinger	Aluminium acetate tartrate s...		3
Caelo	Water	15068702	5
Serumwerk Bernburg AG	Water		2

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Supplier	Substance	Batch	Spectra
Caelo	Water	15287302	1
Caelo	Water	15394202	4
Caelo	Water	15336501	5
Fagron	Water	15F24-T01-023879	7
Fagron	Water	15G09-T02-024364	4
Caelo	Water	15H25-T18-025678	1
Caelo	Water	16127901	2
Caelo	Water	15H25-T14-025670	2
Fagron	Water	15K10-T04-027614	2
Fagron	Water	16F13-T14-034274	1
Wepa	Water	LOTAP0025	1
Caelo	Water	15I10-T08-025964	1
Fagron	Chlorhexidine digluconate so...	11081502	1
Caelo	Chlorhexidine digluconate so...	10213458	1
Caelo	Chlorhexidine digluconate so...	10213441	1
Euro OTC	Chlorhexidine digluconate so...	1206023-02	23
Fagron	Chlorhexidine digluconate so...	1081403	1
Fagron	Chlorhexidine digluconate so...	10031503	1
Euro OTC	Chlorhexidine digluconate so...	1206012-02	1
Hedinger/Sanacorp6.5.2014	Chlorhexidine digluconate so...	1234	1
EuRho	Chlorhexidine digluconate so...	1206023-02	1
Fagron	Chlorhexidine digluconate so...	12K22-N09	17
Fragon	Chlorhexidine digluconate so...	12F01-N21	2
Euro OTC	Chlorhexidine digluconate so...	1308002	2
Fagron	Chlorhexidine digluconate so...	1308002-001	1
Euro OTC	Chlorhexidine digluconate so...	1308002-01	18
Euro OTC	Chlorhexidine digluconate so...	130800201	4
Caelo	Chlorhexidine digluconate so...	1308002	1
Gehe	Chlorhexidine digluconate so...	1308002-01	1
Euro OTC	Chlorhexidine digluconate so...	1308002-02	24
Evonic	Chlorhexidine digluconate so...	1308002-02	2
Gehe	Chlorhexidine digluconate so...	1308002-02	1
Caelo	Chlorhexidine digluconate so...	1308002-02	5
	Chlorhexidine digluconate so...	1308002-02	1
Caelo	Chlorhexidine digluconate so...	13136114	4
Caelo	Chlorhexidine digluconate so...	13081502	1
Caelo	Chlorhexidine digluconate so...	13136105	3
GEHE 20.05.2014	Chlorhexidine digluconate so...	13136114	1
Berkel AHK	Chlorhexidine digluconate so...	13136115	1
Fagron	Chlorhexidine digluconate so...	13D16-N04	9
Caelo	Chlorhexidine digluconate so...	13136115	2
Fagron	Chlorhexidine digluconate so...	13A29-N06	11
AHD	Chlorhexidine digluconate so...	13136115	1
Fagron	Chlorhexidine digluconate so...	13H19-B01	5
Fagron	Chlorhexidine digluconate so...	13H19-B01-285448	3
Fagron	Chlorhexidine digluconate so...	13H19-B01-285449	1
Fagron	Chlorhexidine digluconate so...	13H19-B01-285451	5
Fagron	Chlorhexidine digluconate so...	13H19-B01-285452	4
Fagron	Chlorhexidine digluconate so...	13H19-B01-285453	9
Fagron	Chlorhexidine digluconate so...	13K16B06288853	1
Fagron	Chlorhexidine digluconate so...	13K26-B06	8
Fagron	Chlorhexidine digluconate so...	13k26-b06	1
Fagron	Chlorhexidine digluconate so...	13K26-B06-288848	2
Fagron	Chlorhexidine digluconate so...	13K26-B06289365	1
Fagron	Chlorhexidine digluconate so...	13K26-B06-288849	1
Caelo	Chlorhexidine digluconate so...	13K26-B06-288849	2
PHOENIX 25.07.2014	Chlorhexidine digluconate so...	13k26-b06-288849	1
Fagron	Chlorhexidine digluconate so...	13K26-B06-288853	3
Fagron	Chlorhexidine digluconate so...	13K-26-B06-288853	1
Phönix Gotha	Chlorhexidine digluconate so...	13K26-B06-288853	1

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Supplier	Substance	Batch	Spectra
Hedinger/Sanacorp6.5.2014	Chlorhexidine digluconate so...	13K26-B06289365	1
Fagron	Chlorhexidine digluconate so...	13K26-B06-289365	6
Fagron	Chlorhexidine digluconate so...	13K26-B06-289366	1
Caelo	Chlorhexidine digluconate so...	14011004	2
Sanacorp	Chlorhexidine digluconate so...	14011004	1
Euro OTC	Chlorhexidine digluconate so...	13KB062888448	1
Caelo	Chlorhexidine digluconate so...	14011013	5
Caelo	Chlorhexidine digluconate so...	14011009	1
sanacorp	Chlorhexidine digluconate so...	14011015	1
Caelo	Chlorhexidine digluconate so...	14011017	3
Caelo	Chlorhexidine digluconate so...	14011015	2
Lamotte / Gehe	Chlorhexidine digluconate so...	14011017	1
Caelo	Chlorhexidine digluconate so...	14011018	2
Caelo	Chlorhexidine digluconate so...	14011020	1
Euro OTC	Chlorhexidine digluconate so...	1412018-01	15
EuroPTC/Phönix	Chlorhexidine digluconate so...	1412018-01	1
Phönix Gotha	Chlorhexidine digluconate so...	1412018-01	1
Caelo	Chlorhexidine digluconate so...	1412018-01	3
Euro OTC	Chlorhexidine digluconate so...	141201801	1
Euro OTC	Chlorhexidine digluconate so...	1412018-02	9
Caelo	Chlorhexidine digluconate so...	141201802	2
Eu Rho/ Gehe	Chlorhexidine digluconate so...	1412018-02	1
Euro OTC	Chlorhexidine digluconate so...	141218-01	1
Euro OTC	Chlorhexidine digluconate so...	1412018801	1
Phönix Gotha	Chlorhexidine digluconate so...	14120189-01	1
Caelo	Chlorhexidine digluconate so...	14331301	7
Caelo	Chlorhexidine digluconate so...	14331303	2
Noweda18.12.2014	Chlorhexidine digluconate so...	14331303	1
Caelo	Chlorhexidine digluconate so...	14331307	6
Caelo	Chlorhexidine digluconate so...	14331306	2
Phoenix	Chlorhexidine digluconate so...	14331307	1
Cealo	Chlorhexidine digluconate so...	14331307	1
Caelo	Chlorhexidine digluconate so...	14331309	2
Caelo	Chlorhexidine digluconate so...	14331310	1
Caelo	Chlorhexidine digluconate so...	14331308	1
Caelo	Chlorhexidine digluconate so...	14331312	6
Sanacorp	Chlorhexidine digluconate so...	14331312	1
sanacorp	Chlorhexidine digluconate so...	14331312	1
Caelo	Chlorhexidine digluconate so...	14D25-B04	2
Caelo	Chlorhexidine digluconate so...	14331313	2
Fagron	Chlorhexidine digluconate so...	14D25-B04-294673	4
Fagron	Chlorhexidine digluconate so...	14D25-B04	1
Fagron	Chlorhexidine digluconate so...	14D25-B04-294675	1
Fagron	Chlorhexidine digluconate so...	14D25-B04-294674	2
Fagron	Chlorhexidine digluconate so...	14D25-B04-299288	1
Fagron	Chlorhexidine digluconate so...	15/03-B02-315213	1
Fagron	Chlorhexidine digluconate so...	14D25-B04-299289	1
Caelo	Chlorhexidine digluconate so...	15/03-B02-315552	1
Euro OTC	Chlorhexidine digluconate so...	1508022-01	11
Caelo	Chlorhexidine digluconate so...	1508022-01	3
Euro OTC	Chlorhexidine digluconate so...	1508022-02	4
Euro OTC	Chlorhexidine digluconate so...	150802201	2
Bombastus	Chlorhexidine digluconate so...	1508022-02	1
Caelo	Chlorhexidine digluconate so...	15109201	8
Caelo	Chlorhexidine digluconate so...	1508022-22	1
Euro OTC	Chlorhexidine digluconate so...	1508072-02	1
Caelo	Chlorhexidine digluconate so...	15109202	3
Euro OTC	Chlorhexidine digluconate so...	151103-01	1
Euro OTC	Chlorhexidine digluconate so...	1511033-01	11
Gehe	Chlorhexidine digluconate so...	151103301	1

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Supplier	Substance	Batch	Spectra
Phoenix	Chlorhexidine digluconate so...	1511033-01	1
Fagron	Chlorhexidine digluconate so...	15121406	1
Caelo	Chlorhexidine digluconate so...	15131502	4
Caelo	Chlorhexidine digluconate so...	1511033-01	1
Caelo	Chlorhexidine digluconate so...	15131503	7
Caelo	Chlorhexidine digluconate so...	15131504	9
Geilenkirchen	Chlorhexidine digluconate so...	15131503	1
Sanacorp 17.07.2015	Chlorhexidine digluconate so...	15131504	1
Caelo	Chlorhexidine digluconate so...	15131505	8
Fagron	Chlorhexidine digluconate so...	15131505	2
Caelo	Chlorhexidine digluconate so...	15131508	2
Caelo	Chlorhexidine digluconate so...	15131509	15
Caelo	Chlorhexidine digluconate so...	15131510	6
Noweda	Chlorhexidine digluconate so...	15131510	1
Caelo	Chlorhexidine digluconate so...	15131512	3
Caelo	Chlorhexidine digluconate so...	15131604	1
Caelo	Chlorhexidine digluconate so...	15292504	8
Caleo/Sanacorp	Chlorhexidine digluconate so...	15292507	1
Caelo	Chlorhexidine digluconate so...	15292508	8
Caelo	Chlorhexidine digluconate so...	15292509	1
Noweda	Chlorhexidine digluconate so...	15292508	1
Caelo	Chlorhexidine digluconate so...	15292511	1
Euro OTC	Chlorhexidine digluconate so...	1529508	1
Caelo	Chlorhexidine digluconate so...	1529511	1
Fagron	Chlorhexidine digluconate so...	15C03B02	2
Schütz Dishman Biotech ...	Chlorhexidine digluconate so...	15E13-B07	1
Fagron	Chlorhexidine digluconate so...	15C03-B02-306308	1
Fragon/ Phönix	Chlorhexidine digluconate so...	15C03-B02-306308	1
Fagron	Chlorhexidine digluconate so...	15E13-B07-309826	2
Fagron	Chlorhexidine digluconate so...	15F30B05	1
Fagron	Chlorhexidine digluconate so...	15E13B07309826	1
Fagron	Chlorhexidine digluconate so...	15F30-B05	2
Fagron	Chlorhexidine digluconate so...	15F30-B05-309827	1
Caelo	Chlorhexidine digluconate so...	15F30-B05-311700	1
Schütz Dishman Biotech ...	Chlorhexidine digluconate so...	15I03-B02	1
Fagron	Chlorhexidine digluconate so...	15I03B02314176	1
Caelo	Chlorhexidine digluconate so...	15I03-B02-315213	4
Fagron	Chlorhexidine digluconate so...	15I03-B02-313663	1
Fagron	Chlorhexidine digluconate so...	15I03-B02-315552	2
Fagron	Chlorhexidine digluconate so...	15J03-B02	1
Caelo	Chlorhexidine digluconate so...	16002501	8
Fagron	Chlorhexidine digluconate so...	15I03B02317319	1
Caelo	Chlorhexidine digluconate so...	16002505	3
Caesar & Loretz	Chlorhexidine digluconate so...	16002510	1
Caelo	Chlorhexidine digluconate so...	16002506	1
Caelo	Chlorhexidine digluconate so...	16002510	1
Caelo	Chlorhexidine digluconate so...	16308801	4
Fagron	Chlorhexidine digluconate so...	16B25-B98-318800	1
Fagron	Chlorhexidine digluconate so...	16B25-B98-318799	1
Caelo	Chlorhexidine digluconate so...	16E09-B03	1
Fagron	Chlorhexidine digluconate so...	16E09-B03-323873	1
Evonik	Chlorhexidine digluconate so...	3896220404	1
Fagron	Chlorhexidine digluconate so...	2614Q-01262	1
Fagron	Chlorhexidine digluconate so...	26091402	1
Fagron	Chlorhexidine digluconate so...	BK13-CG-018	2
Fagron	Chlorhexidine digluconate so...	BK13-CG-285447	1
Fagron	Chlorhexidine digluconate so...	BK14-CG-003	2
GEHE 08.12.2014	Chlorhexidine digluconate so...	BK14-CG-003	1
Fagron	Chlorhexidine digluconate so...	BK15-CG-001	3
Fagron	Chlorhexidine digluconate so...	BK14-CG-023	1

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Supplier	Substance	Batch	Spectra
Fagron	Chlorhexidine digluconate so...	4111303	1
Fagron	Chlorhexidine digluconate so...	103311262	1
Fagron	Chlorhexidine digluconate so...	204211262	1
Euro OTC	Chlorhexidine digluconate so...	106023-02	1
Fagron	Chlorhexidine digluconate so...	6111210	1
Fagron	Chlorhexidine digluconate so...	BK16-CG-005	1
Euro OTC	Chlorhexidine digluconate so...	1105012-01	2
Fagron	Chlorhexidine digluconate so...	9081302	1
Caelo	Chlorhexidine digluconate so...	10200303	1
EuRho	Chlorhexidine digluconate so...	1105012-01	1
Celo	Chlorhexidine digluconate so...	110816-7	1
Gehe	Chlorhexidine digluconate so...	1110012-01	1
Caelo	Chlorhexidine digluconate so...	11135107	1
Gehe	Chlorhexidine digluconate so...	11135114	2
Caelo	Chlorhexidine digluconate so...	11135114	2
Phönix, 17.10.2012	Chlorhexidine digluconate so...	1110012-01	1
Euro OTC	Chlorhexidine digluconate so...	1110012-01	1
Caelo	Chlorhexidine digluconate so...	11353001	3
Noweda	Chlorhexidine digluconate so...	11353004	1
Caelo	Chlorhexidine digluconate so...	11353004	4
Caelo	Chlorhexidine digluconate so...	11353009	2
Phönix	Chlorhexidine digluconate so...	11353004	1
Caelo	Chlorhexidine digluconate so...	11353012	3
Anzag 21.12.12	Chlorhexidine digluconate so...	11353012	2
ANZAG	Chlorhexidine digluconate so...	11353012	1
Caelo	Chlorhexidine digluconate so...	11353013	5
Noweda	Chlorhexidine digluconate so...	11353013	1
Fagron	Chlorhexidine digluconate so...	11K09-N05	4
Caelo	Chlorhexidine digluconate so...	11L05-N08	1
Fagron	Chlorhexidine digluconate so...	11L05-N08	4
Fagron	Chlorhexidine digluconate so...	11L05-N080069/262	1
Phoenix 17.07.2012	Chlorhexidine digluconate so...	1202010-01	2
Euro OTC	Chlorhexidine digluconate so...	1202010-01	10
Noweda	Chlorhexidine digluconate so...	1202010-01	3
Fagron	Chlorhexidine digluconate so...	120201001	1
Phönix/EuRho	Chlorhexidine digluconate so...	1206023-01	2
Euro OTC	Chlorhexidine digluconate so...	1206023-01	13
Euro OTC	Chlorhexidine digluconate so...	120602301	3
Alliance Healthcare	Chlorhexidine digluconate so...	1206023	1
Fagron	Chlorhexidine digluconate so...	120355-ooo4	1
Sanacorp	Chlorhexidine digluconate so...	1206023-01	1
Phönix	Chlorhexidine digluconate so...	1206023-01	1
Caelo	Chlorhexidine digluconate so...	1206023-01	1
Anzag	Chlorhexidine digluconate so...	1206023-01	1
10.05.2013	Chlorhexidine digluconate so...	1206023-01	1
Gehe	Chlorhexidine digluconate so...	1206023-01	1
Gehe	Chlorhexidine digluconate so...	1206023-02	7
Caelo	Chlorhexidine digluconate so...	1206023-02	1
Phönix	Chlorhexidine digluconate so...	1206023-02	2
Phönix 28.01.2014	Chlorhexidine digluconate so...	1206023-02	1
Caelo	Chlorhexidine digluconate so...	12114001	5
Noweda	Chlorhexidine digluconate so...	12114001	1
Gehe	Chlorhexidine digluconate so...	12114001	1
Caelo	Chlorhexidine digluconate so...	12114007	1
Sanacorp	Chlorhexidine digluconate so...	12114001	1
Fagron	Chlorhexidine digluconate so...	12114007	1
Caelo	Chlorhexidine digluconate so...	12114008	5
Caelo	Chlorhexidine digluconate so...	12114012	10
Gehe	Chlorhexidine digluconate so...	12114012	1
Noweda	Chlorhexidine digluconate so...	12114012	1

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Supplier	Substance	Batch	Spectra
AHD	Chlorhexidine digluconate so...	12114012	1
Gehe	Chlorhexidine digluconate so...	12114014	1
Caelo	Chlorhexidine digluconate so...	12114015	2
Caelo	Chlorhexidine digluconate so...	12114013	1
Caelo	Chlorhexidine digluconate so...	12114014	5
Caelo	Chlorhexidine digluconate so...	12114019	3
Fagron	Chlorhexidine digluconate so...	1213E-01262	1
Fagron	Chlorhexidine digluconate so...	12a02-n11	1
Fagron	Chlorhexidine digluconate so...	12A02-N11	6
Phönix Gotha	Chlorhexidine digluconate so...	12A02-N11	1
Fagron	Chlorhexidine digluconate so...	12F01-N021	1
Fagron	Chlorhexidine digluconate so...	12F01-N21	39
Fargon	Chlorhexidine digluconate so...	12F01-N21	1
Großhandel	Chlorhexidine digluconate so...	12F01-N21	1
Fargon/ Noweda	Chlorhexidine digluconate so...	12f01n21	1
Fagron	Chlorhexidine digluconate so...	12f01-N21	1
Caelo	Chlorhexidine digluconate so...	12H14-N016	1
Fagron	Chlorhexidine digluconate so...	12H14-N06	22
Caelo	Chlorhexidine digluconate so...	12H14-N06	2
Phönix	Chlorhexidine digluconate so...	12H14-N06	1
Fagron	Chlorhexidine digluconate so...	12H-14-N06	1
Phönix Gotha	Chlorhexidine digluconate so...	12H14-N06	1
Gehe	Chlorhexidine digluconate so...	12h14-n06	1
Fagron	Chlorhexidine digluconate so...	12H14N06	1
ANZAG 27.12.2012	Chlorhexidine digluconate so...	12H14No6	1
Fagron	Chlorhexidine digluconate so...	12H14-No6	4
Fagron	Chlorhexidine digluconate so...	12H14-No06	1
Sanacorp	Chlorhexidine digluconate so...	12K22-N09	1
Fagron	Chlorhexidine digluconate so...	12K22-0005	1
Caelo	Chlorhexidine digluconate so...	12k22-n09	1
Euro OTC	Chlorhexidine digluconate so...	12K22-N09	1
Fagron	Chlorhexidine digluconate so...	12K22-No9	1
Euro OTC	Chlorhexidine digluconate so...	130002-01	1
Fagron	Chlorhexidine digluconate so...	13081204	1
Caelo	Chlorhexidine digluconate so...	13136103	14
Caelo	Chlorhexidine digluconate so...	13136101	1
Caelo	Chlorhexidine digluconate so...	13136015	1
Sanacorp	Chlorhexidine digluconate so...	13136103	1
Gehe	Chlorhexidine digluconate so...	13136105	1
Caelo	Chlorhexidine digluconate so...	13136112	2
Caelo	Chlorhexidine digluconate so...	13A29-N06	1
Sanacorp	Chlorhexidine digluconate so...	13136115	2
Caelo	Chlorhexidine digluconate so...	1316103	1
Cael/Nowda	Chlorhexidine digluconate so...	13136115	1
Phönix Gotha	Chlorhexidine digluconate so...	13A29-N06	1
Fagron	Chlorhexidine digluconate so...	13D16-N040090/192	1
Fagron	Chlorhexidine digluconate so...	13A29-N060155/228	1
Klenk	Chlorhexidine digluconate so...	13D16-N04	1
Fagron	Chlorhexidine digluconate so...	13d16-N04	2
Euro OTC	Chlorhexidine digluconate so...	13D16-N04	1
Fagron	Chlorhexidine digluconate so...	13H19B01	1
Großhandel	Chlorhexidine digluconate so...	13H19-B01	1
Fagron	Chlorhexidine digluconate so...	13H19-B01-285447	2
Fagron	Chlorhexidine digluconate so...	13h19b01285447	1
Caelo	Chlorhexidine digluconate so...	13H19-B01-285451	1
Fagron	Chlorhexidine digluconate so...	13H19B01285451	1
Phoenix	Chlorhexidine digluconate so...	13H19-B01-285452	1
Caelo	Chlorhexidine digluconate so...	13k26-b06-28884	1
Caelo	Chlorhexidine digluconate so...	14011011	1
Fagron	Chlorhexidine digluconate so...	15103B02-315212	1

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Supplier	Substance	Batch	Spectra
Fagron	Chlorhexidine digluconate so...	17011310	1
Caelo	Chlorhexidine digluconate so...	20031301	1
Fagron	Chlorhexidine digluconate so...	25051304	1
Fagron	Chlorhexidine digluconate so...	23121307	1
Fagron	Chlorhexidine digluconate so...	20200112-1	1
Fagron	Chlorhexidine digluconate so...	2612M01262	1
Fagron	Chlorhexidine digluconate so...	2512M01262	1
Caelo	Chlorhexidine digluconate so...	32/AD1	1
Caelo	Chlorhexidine digluconate so...	BK13-CG-011	1
Euro OTC	Chlorhexidine digluconate so...	282215	1
Euro OTC	Chlorhexidine digluconate so...	3896220404	1
Fagron	Chlorhexidine digluconate so...	BK13-CG-011	2
Fagron	Chlorhexidine digluconate so...	4513U1262	1
Caelo	Chlorhexidine digluconate so...	1202010-01	1
Caelo	Chlorhexidine digluconate so...	11L05-N080040	1
Fiebig	Chlorhexidine digluconate so...	1110012-01	1
AHD	Chlorhexidine digluconate so...	1206023-02	3
Fagron	Chlorhexidine digluconate so...	12A02-11	1
Phönix	Chlorhexidine digluconate so...	13K26-B06-28965	1
Hedinger / Gehe	Aluminium acetate tartrate s...	20155B	1
Euro OTC	Aluminium acetate tartrate s...	20157B	1
Caelo	Aluminium acetate tartrate s...	110024	1
Dr. Seeger GmbH/Noweda	Aluminium acetate tartrate s...	20146B	1
Phönix	Aluminium acetate tartrate s...	20150B	1
hedinger/anzag	Aluminium acetate tartrate s...	20152B	1
Hedinger/AHD	Aluminium acetate tartrate s...	20146B	1
Anzag/ Hedinger	Aluminium acetate tartrate s...	20153B	1
Hedinger/ Sanacorp	Aluminium acetate tartrate s...	20150B	1
Franz GmbH	Aluminium acetate tartrate s...	20153B	1
Hedinger/Phoenix	Aluminium acetate tartrate s...	20154B	1
Hedinger / Gehe	Aluminium acetate tartrate s...	20154B	1
Caelo	Aluminium acetate tartrate s...	4071201	1
Hedinger	Aluminium acetate tartrate s...	1002211793	1
Phönix Gotha	Aluminium acetate tartrate s...	12116803	1
Caelo	Aluminium acetate tartrate s...	10114803	1
Caelo	Aluminium acetate tartrate s...	12116802	1
Phönix Gotha	Aluminium acetate tartrate s...	11315007	2
Alliance Healthcare	Aluminium acetate tartrate s...	12318705	2
Caelo	Aluminium acetate tartrate s...	13101105	1
Hedinger/Phönix	Aluminium acetate tartrate s...	20155B	1
Hedinger/Phönix	Aluminium acetate tartrate s...	20157B	2
Caelo	Aluminium acetate tartrate s...	13378706	2
Hedinger/AHD	Aluminium acetate tartrate s...	20152B	2
Hedinger/Holdermann	Aluminium acetate tartrate s...	20150B	1
Franz GmbH / Phoenix	Aluminium acetate tartrate s...	20153B	1
Hedinger Phönix	Aluminium acetate tartrate s...	20153B	1
Hedinger/AHD	Aluminium acetate tartrate s...	201153B	1
Caesar & Lorenz	Aluminium acetate tartrate s...	12318703	1
Industries AG / Phoenix	Chlorhexidine digluconate so...	1308002-02	1
Fagron	Chlorhexidine digluconate so...	15/03-B02-313663	1
A.H.D.	Chlorhexidine digluconate so...	1206023-01	3
Caelo	Chlorhexidine digluconate so...	15292507	1
Fagron	Chlorhexidine digluconate so...	16E09-B03-320995	1
Caelo	Chlorhexidine digluconate so...	1206023-02-335731907	1
Caelo	Chlorhexidine digluconate so...	12122222	1
Fagron	Water	14E30-T11-012852	1
Caelo	Water	14321201	1
Fagron	Water	14F02-T03-012891	1
Caelo	Water	14364201	1
Fagron	Water	14H21-T05-014956	1

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Supplier	Substance	Batch	Spectra
Phönix Gotha	Water	14K05-T02-016775	2
Fagron	Water	14K05-T02-016775	2
Fagron	Water	14K05-T03-016779	1
Fresenius	Water	14KB1003	1
Fagron	Water	14L03-T09-017794	2
Fagron	Water	14L03-T07-017788	2
Fagron	Water	14L03-T03-017773	1
Rabenapotheke	Water	14L03-T11-017800	1
Fagron	Water	14L03T09017794	1
Fagron	Water	15/10-T08-025964	1
Fagron	Water	15/10-T09-025968	1
Caelo	Water	15013201	1
Phönix Gotha	Water	15019101	3
Caelo	Water	15068701	1
Caelo	Water	15220601	3
Caelo	Water	15220602	2
Phönix Gotha	Water	15142501	1
Phönix Gotha	Water	15235201	2
Caelo	Water	1524101	1
Phönix Gotha	Water	15253901	1
Caelo	Water	15253901	2
Caelo	Water	15254101	3
Caelo	Water	15287401	2
Caelo	Water	15287501	2
Caelo	Water	15355401	1
Caelo	Water	153712002	1
Caelo	Water	15371202	3
Caesar & Loretz GmbH Hi...	Water	15394202	1
Caelo	Water	15394201	1
Fagron	Water	15D13-T09-021469	5
Caelo	Water	1542701	1
Caelo	Water	15394501	2
Caelo	Water	15427201	2
Klenk	Water	15D14-T-021499	1
Fagron	Water	15D14-T05-021481	1
Fagron	Water	15D14-T05	2
Fagron	Water	15D14-T09-021490	2
Fagron	Water	15D14-T06-021484	1
Fagron	Water	15D14-T10-021493	4
Fagron	Water	15D14-T13-021499	1
Fagron	Water	15D14-T14-021502	3
Noweda	Water	15F04-T03-023259	1
Fagron	Water	15F04-T05-023263	3
Fagron	Water	15F04-T03-023529	1
Caelo	Water	15F04-T03-23259	1
Caelo	Water	15F04-T05-023263	1
Fargon/Kehr	Water	15F04-T05-023263	1
Fagron	Water	15F24T03-023883	1
Caelo	Water	15F24-T03-023883	2
Fagron	Water	15G09-T04-024368	1
Fagron	Water	15h0-T09-025968	1
Fagron	Water	15H25-T14-025670	3
Fagron	Water	15H25-T18-025678	1
Fagron	Water	15H25-T16-025674	1
Caelo	Water	15H25-T21-025683	1
Fagron	Water	15H25-T21-025683	3
Ebert 04.04.2014	Water	15K10-T04-027614	1
Fagron	Water	15K10-T06-027620	1
Fagron	Water	15L14-T14-028664	4
Phoenix	Water	15L14-T14	1

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Supplier	Substance	Batch	Spectra
Caelo	Water	15K10-T06-027620	1
Fagron	Water	15L15-T01-028672	2
Fargon/Noweda	Water	15L15-T028676	1
Fagron	Water	15L15-T03-028676	1
Fagron	Water	15L15-T05-028681	1
Phoenix	Water	15L15-T07	1
Kehr	Water	16006001	2
Caelo	Water	16065101	1
Caelo	Water	16065601	1
Caelo	Water	16093301	2
Caelo	Water	16065001	1
Caesar & Loretz GmbH Hi...	Water	16127902	1
Caelo	Water	16151201	1
Caelo	Water	16223601	2
Caelo	Water	16178101	1
Caelo	Water	1615201	1
Caelo	Water	16286801	1
Caelo	Water	16255201	1
Fagron	Water	16C22-T09-031414	3
Fagron	Water	16C23-T06-031423	2
Caelo	Water	16C23-/08031427	1
Caelo	Water	16313201	1
Caelo	Water	16C23-T16-031436	1
Fagron	Water	16F13-T11-034264	4
Caelo	Water	17011603	1
Caelo	Water	AP0026	1
Caelo	Water	16F14-T07-034326	1
Hedinger/ Sanacorp	Water	AP0022	1
Caelo	Water	23081606	1
Wepa	Water	AP0024	1
WEPA	Water	LOTAP0012	2
Wepa	Water	LOTAP0015	1
Caelo	Water		1
Caelo	Water	LOTAP0025	1
Wepa	Water	LOTAP0020	1
Wepa	Water	LOTAP0017	1
WEPA	Water	LOTAP0025	2
Rondell Apotheke	Water	LOTAP0016	1
Wepa	Water	LOTAP0035	1
WEPA/Noweda	Water	LOTAP0033	1
Wepa	Water	LOTAP0013	1
Wepa/ Noweda	Water	LOTAP0038	1

- 57 052 spectra from 332 *Apo-Ident* customers from a total of 19 681 batches from a further 326 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	690	0	33 654
Type B	0	695	0	62 133
Type C	0	1310	79	56 798

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 % (> 99.9689 %)	100.0000 % (> 99.1304 %)
Type B	100.0000 % (> 99.9722 %)	100.0000 % (> 99.1367 %)
Type C	100.0000 % (> 99.6088 %)	94.3125 % (> 94.0965 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30869	31342	5.61	21.33
31057	32354	2.87	35.76
31240	31735	3.41	36.93
31342	31342	0.00	25.51
31463	31463	0.00	40.12
31624	31718	1.94	38.84
31676	32354	4.06	35.14
31705	31718	9.91	31.18
31718	31718	0.00	39.73
31735	31735	0.00	38.42
31809	31718	4.79	38.91
31829	31463	4.56	35.96
31846	31846	0.00	41.32
31959	31342	5.66	22.65
32308	31718	9.90	32.45
32354	32354	0.00	37.89
32732	31735	2.93	38.31
32831	32831	0.00	35.97

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Wines**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30641-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Wines; Chest elixir; Condurango wine; Elixir e succo liquiritiae; Fortified wine; Gel basis Audor®; Liquiritiae succi elixir; Liquiritiae succus depur. Solut.; Liquorice juice, purified; Pepsin wine; Succus liquiritiae depur. solut.; Vinum condurangum; Vinum pepsini

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Wines*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor	Gel basis Audor®	AP111500	30641	40	20101104
Caelo	Condurango wine	11239009	30901	50	20110909
Caelo	Pepsin wine	12277403	30902	60	20120921
Audor	Gel basis Audor®	AP103113G	31108	40	1404231

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fortified wine	13208302	31127	40	1403400
Caelo	Chest elixir	13003109	31213	40	1405332
Caelo	Fortified wine	13208306	31222	70	20130822
Caelo	Fortified wine	13397204	31466	40	20131216
Caelo	Pepsin wine	14339802	31569	30	1503624
Caelo	Condurango wine	14345603	31581	40	1505325
Caelo	Chest elixir	14182707	31615	40	20140709
Caelo	Liquorice juice,...	14203111	31652	40	20140711
Caelo	Pepsin wine	15449301	31849	40	20160118
Caelo	Liquorice juice,...	162291	32700	40	20160824*
Audor	Gel basis Audor®	AP53801G	32724	40	20151012
Audor	Gel basis Audor®	AP63101G	32751	40	20160906

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 690 spectra of 16 reference samples from the substance/substance group *Wines*. These samples are listed above in the [calibration samples](#) section.
- 33 654 spectra from a total of 782 batches from further 219 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 516 spectra of 17 reference samples from the substance/substance group *Wines*.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Gel basis Audor®	pending	30172	40
Caelo	Fortified wine	10208202	30186	31
Caelo	Liquorice juice, purified	11293204	30415	40
Caelo	Chest elixir	12041501	30504	40
Audor Pharma	Gel basis Audor®	AP103081G	30607	40
Caelo	Condurango wine	11239009	30901 [†]	10
Caelo	Fortified wine	13397204	31466 [†]	20
Caelo	Pepsin wine	14339802	31569 [†]	15

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

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Condurango wine	14345603	31581 [†]	20
Caelo	Chest elixir	14182707	31615 [†]	20
Caelo	Liquorice juice, purified	14203111	31652 [†]	20
Caelo	Pepsin wine	15449301	31849 [†]	20
Caelo	Pepsin wine	15449303	32076	40
Caelo	Liquorice juice, purified	161241	32200	40
Caelo	Fortified wine	161795	32336	40
Audor Pharma	Gel basis Audor [®]	AP63101G	32752	40
Caelo	Chest elixir	15379113	32956	40

- 63 078 spectra from a total of 1461 batches from further 434 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.

- 96 spectra from 28 *Apo-Ident* customers from 46 batches from the substance/substance group *Wines*.

Supplier	Substance	Batch	Spectra
Caelo	Fortified wine	15175501	1
Caelo	Fortified wine	12059809	2
Caelo	Fortified wine	12059810	1
Audor Pharma	Gel basis Audor [®]	AP100852	1
Audor Pharma	Gel basis Audor [®]	AP100852G	4
Audor Pharma	Gel basis Audor [®]	Ap103081G	1
Caelo	Chest elixir	18101306	1
Caelo	Chest elixir	12091406	1
Caelo	Chest elixir	3031506	1
Caelo	Chest elixir	19071402	1
Caelo	Condurango wine	14345604	1
Audor Pharma	Gel basis Audor [®]	102464	4
Audor Pharma	Gel basis Audor [®]		12
Audor Pharma	Gel basis Audor [®]	AP102464	1
Audor Pharma	Gel basis Audor [®]	AP102464G	4
Audor Pharma	Gel basis Audor [®]	AP103993G	3
Audor Pharma	Gel basis Audor [®]	AP53801G	3
Fagron	Gel basis Audor [®]	AP103993G	1
Audor Pharma	Gel basis Audor [®]	ap103113g	1
Anzag	Gel basis Audor [®]	103081G	1
Caelo	Gel basis Audor [®]	18041301	1
Audor Pharma	Gel basis Audor [®]	AP103081G	2
Audor Pharma	Gel basis Audor [®]	AP103081	1
Großhandel	Gel basis Audor [®]	AP100852G	1
Audor Pharma	Gel basis Audor [®]	AP103113G	1
Fiebig	Chest elixir	11019106	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
Caelo	Liquorice juice, purified	13067606	2
Caelo	Liquorice juice, purified	14002602	4
Caelo	Liquorice juice, purified	13133803	2
Caelo	Liquorice juice, purified	14203104	1
Caelo	Liquorice juice, purified	14203105	3
Caelo	Liquorice juice, purified	14002604	1
Caelo	Liquorice juice, purified	14203107	1
Fagron	Liquorice juice, purified	15155302	2
Caelo	Liquorice juice, purified	14203108	1
Caelo	Liquorice juice, purified	15155302	1
Jenne	Liquorice juice, purified	16124103	1
Caelo	Liquorice juice, purified	11293204	3
Caelo	Liquorice juice, purified	11293208	3
VDL	Liquorice juice, purified	11293210	1
Caelo	Liquorice juice, purified	12061203	1
Caelo	Liquorice juice, purified	12116703	2
VDL	Liquorice juice, purified	12116703	2
Caelo	Liquorice juice, purified	12116704	4
Caelo	Liquorice juice, purified	13067602	2
Caelo	Liquorice juice, purified	12116709	1
Caelo	Liquorice juice, purified	13133801	3
Caelo	Liquorice juice, purified	13067604	1
Caelo	Liquorice juice, purified	1367604	1
Caelo	Liquorice juice, purified	1367605	1

- 58 345 spectra from 332 *Apo-Ident* customers from a total of 20 046 batches from a further 324 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 *Wines* 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 *Wines* 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	690	0	33 654
Type B	0	505	11	62 917
Type C	0	77	19	58 316

The substance/substance group *Wines* 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 % (> 99.9689 %)	100.0000 % (> 99.1304 %)
Type B	100.0000 % (> 99.9719 %)	97.8682 % (> 97.2868 %)
Type C	100.0000 % (> 99.5966 %)	80.2083 % (> 77.0833 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30641	31108	6.68	24.86
30901	31581	10.60	26.93
30902	31569	3.97	27.77
31108	31108	0.00	30.10
31127	31127	0.00	25.21
31213	31213	0.00	38.35
31222	31127	2.16	25.24
31466	31127	3.29	26.96
31569	31569	0.00	28.64
31581	31581	0.00	31.98
31615	31213	8.94	32.64
31652	31127	19.57	34.79
31849	31569	2.09	27.68
32700	32700	0.00	49.06
32724	31127	9.37	27.82
32751	31127	9.03	22.60

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Wood oils**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30710-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Wood oils; Juniper wood oil; Juniperi ligni etheroleum; Oleum Juniperi e Ligno pro uso externo; Oleum terebinthinae rectificat.; Turpentine oil of the maritime pine type

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Wood oils*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Juniper wood oil	11363504	30710	40	20111221
Caelo	Juniper wood oil	11363507	30860	40	20111221
Caelo	Juniper wood oil	13196208	31201	40	1405102
Caelo	Turpentine oil o...	12383210	31214	40	1407275
Euro OTC	Turpentine oil o...	1312026-01	31531	40	20140113
Euro OTC	Turpentine oil o...	1511012	31815	40	20151214*
Euro OTC	Turpentine oil o...	1703005	33232	40	20170327*

Validation samples

A total of 156379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Wood oils*. These samples are listed above in the [calibration samples](#) section.
- 34064 spectra from a total of 791 batches from further 223 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 123 spectra of 4 reference samples from the substance/substance group *Wood oils*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Turpentine oil of the mariti...	10016709	30188	43
Euro OTC	Turpentine oil of the mariti...	1312026-01	31531 [†]	20
Euro OTC	Turpentine oil of the mariti...	1511012	31815 [†]	20
Caelo	Turpentine oil of the mariti...	161997	32317	40

- 63471 spectra from a total of 1473 batches from further 439 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.

- 58 spectra from 42 *Apo-Ident* customers from 31 batches from the substance/substance group *Wood oils*.

*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.

[†]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*.

Supplier	Substance	Batch	Spectra
Caelo	Juniper wood oil	14008301	1
Caelo	Turpentine oil of the mariti...	15185106	1
Caelo	Turpentine oil of the mariti...	15185101	2
Caelo	Turpentine oil of the mariti...	11127908	2
Phönix	Turpentine oil of the mariti...	13378804	1
Euro OTC	Turpentine oil of the mariti...	1210016-01	4
Caelo	Turpentine oil of the mariti...	13378804	1
Caelo	Turpentine oil of the mariti...	12383210	3
Caelo	Turpentine oil of the mariti...	14012601	2
Caelo	Turpentine oil of the mariti...	1424703	1
Euro OTC	Turpentine oil of the mariti...	1407037-01	1
Caelo	Turpentine oil of the mariti...	14242703	1
Caelo	Turpentine oil of the mariti...	412M-02022	1
Euro OTC	Turpentine oil of the mariti...	711Q-03557	1
Schiele	Turpentine oil of the mariti...	55379	1
Caelo	Turpentine oil of the mariti...	11358903	4
Caelo	Turpentine oil of the mariti...	10296303	1
Caelo	Turpentine oil of the mariti...	11127905	1
Caelo	Turpentine oil of the mariti...	11358910	8
Sanacorp	Turpentine oil of the mariti...	12383210	1
Caelo	Turpentine oil of the mariti...	12383201	1
Caelo	Turpentine oil of the mariti...	13106701	6
AHC 20.07 13 250ml	Turpentine oil of the mariti...	13106701	1
Sanacorp	Turpentine oil of the mariti...	13106701	1
Caelo	Turpentine oil of the mariti...	14071201	1
Caelo	Turpentine oil of the mariti...	19061310	1
Caelo	Turpentine oil of the mariti...	24544454	1
Caelo	Juniper wood oil	12342604	1
Caelo	Juniper wood oil	14008303	1
Caelo	Juniper wood oil	11379007	1
Caelo	Juniper wood oil	14008306	1
Taoasis GmbH	Juniper wood oil	736525-110967	1
Taoasis GmbH	Juniper wood oil	604898-109389	1
Caelo	Juniper wood oil		1
Caelo	Juniper wood oil	11363507	1

- 58 383 spectra from 332 *Apo-Ident* customers from a total of 20 064 batches from a further 327 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 *Wood oils* 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 *Wood oils* 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	34 064
Type B	0	99	24	63 471
Type C	0	48	10	58 383

The substance/substance group *Wood oils* 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 % (> 99.9689 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9710 %)	80.4878 % (> 78.0488 %)
Type C	100.0000 % (> 99.5964 %)	82.7586 % (> 77.5862 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30710	31201	3.36	20.64
30860	31201	5.03	22.76
31201	31201	0.00	18.87
31214	31214	0.00	22.74
31531	31214	2.72	23.49
31815	31815	0.00	25.68
33232	33232	0.00	26.50

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Wool alcohol cream DAB/SR
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30425-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Wool alcohol cream DAB/SR; Lanae alcoholum unguentum aquosum DAB/SR; Unguentum alcoholum lanae aquosum DAB/SR

Special notes

When selecting the *Wool alcohol cream DAB/SR* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Wool alcohol cream DAB/SR*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Wool alcohol cre...	13272603	31229	70	20130829
Caelo	Wool alcohol cre...	13369401	31248	40	20131111
Bombastus	Wool alcohol cre...	284945	31271	40	1406054
Caelo	Wool alcohol cre...	13369401	31287	40	1406055
Caelo	Wool alcohol cre...	14031601	31447	40	1512182

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Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Wool alcohol cre...	13394101	31455	30	1509376
Caelo	Wool alcohol cre...	14126801	31481	40	20140415
Caelo	Wool alcohol cre...	153608	31923	40	20151029*
Caelo	Wool alcohol cre...	153609	31926	40	20151103*
Caelo	Wool alcohol cre...	153611	31928	40	20151106*
Caelo	Wool alcohol cre...	153613	31930	40	20151106*
Caelo	Wool alcohol cre...	153615	31933	40	20151029*
Caelo	Wool alcohol cre...	153616	31934	40	20151029*
Caelo	Wool alcohol cre...	153617	31937	40	20151103*
Caelo	Wool alcohol cre...	160901	32160	40	20160414*
Caelo	Wool alcohol cre...	170396	33140	40	20170214*

Validation samples

A total of 156 379 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 660 spectra of 16 reference samples from the substance/substance group *Wool alcohol cream DAB/SR*. These samples are listed above in the [calibration samples](#) section.
- 33 684 spectra from a total of 783 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 2820 spectra of 70 reference samples from the substance/substance group *Wool alcohol cream DAB/SR*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Wool alcohol cream DAB/SR	11140801	30317	40
Caelo	Wool alcohol cream DAB/SR	11171701	30405	40
Bombastus	Wool alcohol cream DAB/SR	263268	30425	40
Caelo	Wool alcohol cream DAB/SR	12066203	30501	40
Caelo	Wool alcohol cream DAB/SR	12066202	30614	40
Bombastus	Wool alcohol cream DAB/SR	270036	30625	40
Bombastus	Wool alcohol cream DAB/SR	265302	30627	40
zu erfassen	Wool alcohol cream DAB/SR	pending	30649	40

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

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Wool alcohol cream DAB/SR	12205402	30655	40
Caelo	Wool alcohol cream DAB/SR	12036401	30656	40
apomix	Wool alcohol cream DAB/SR	39A100412	30676	40
Caelo	Wool alcohol cream DAB/SR	153608	31923 [†]	20
Caelo	Wool alcohol cream DAB/SR	153608	31924	60
Caelo	Wool alcohol cream DAB/SR	153608	31925	60
Caelo	Wool alcohol cream DAB/SR	153609	31926 [†]	20
Caelo	Wool alcohol cream DAB/SR	153610	31927	60
Caelo	Wool alcohol cream DAB/SR	153611	31928 [†]	20
Caelo	Wool alcohol cream DAB/SR	153612	31929	60
Caelo	Wool alcohol cream DAB/SR	153613	31930 [†]	20
Caelo	Wool alcohol cream DAB/SR	153614	31931	60
Caelo	Wool alcohol cream DAB/SR	153615	31932	60
Caelo	Wool alcohol cream DAB/SR	153615	31933 [†]	20
Caelo	Wool alcohol cream DAB/SR	153616	31934 [†]	20
Caelo	Wool alcohol cream DAB/SR	153616	31935	60
Caelo	Wool alcohol cream DAB/SR	153617	31936	60
Caelo	Wool alcohol cream DAB/SR	153617	31937 [†]	20
Caelo	Wool alcohol cream DAB/SR	160078	32157	40
Caelo	Wool alcohol cream DAB/SR	160899	32158	40
Caelo	Wool alcohol cream DAB/SR	160900	32159	40
Caelo	Wool alcohol cream DAB/SR	160902	32161	40
Caelo	Wool alcohol cream DAB/SR	160903	32162	40
Caelo	Wool alcohol cream DAB/SR	160904	32163	40
Caelo	Wool alcohol cream DAB/SR	160905	32164	40
Caelo	Wool alcohol cream DAB/SR	160906	32165	40
Caelo	Wool alcohol cream DAB/SR	160907	32166	40
Caelo	Wool alcohol cream DAB/SR	161122	32167	40
Caelo	Wool alcohol cream DAB/SR	160143	32295	40
Caelo	Wool alcohol cream DAB/SR	161208	32296	40
Caelo	Wool alcohol cream DAB/SR	161578	32361	40
Caelo	Wool alcohol cream DAB/SR	161578	32362	40
Caelo	Wool alcohol cream DAB/SR	161577	32363	40
Caelo	Wool alcohol cream DAB/SR	161579	32364	40
Caelo	Wool alcohol cream DAB/SR	161580	32365	40
Caelo	Wool alcohol cream DAB/SR	161580	32366	40
Caelo	Wool alcohol cream DAB/SR	161581	32367	40
Caelo	Wool alcohol cream DAB/SR	161577	32379	40
Caelo	Wool alcohol cream DAB/SR	161776	32380	40
Caelo	Wool alcohol cream DAB/SR	161774	32381	40
Caelo	Wool alcohol cream DAB/SR	161778	32513	40
Caelo	Wool alcohol cream DAB/SR	162490	32514	40
Caelo	Wool alcohol cream DAB/SR	161578	32630	40
Caelo	Wool alcohol cream DAB/SR	161579	32631	40
Caelo	Wool alcohol cream DAB/SR	161992	32632	40
Caelo	Wool alcohol cream DAB/SR	161992	32633	40
Caelo	Wool alcohol cream DAB/SR	161992	32634	40
Caelo	Wool alcohol cream DAB/SR	161993	32635	40
Caelo	Wool alcohol cream DAB/SR	161993	32636	40
Caelo	Wool alcohol cream DAB/SR	161993	32637	40
Caelo	Wool alcohol cream DAB/SR	161994	32638	40
Caelo	Wool alcohol cream DAB/SR	161994	32639	40
Caelo	Wool alcohol cream DAB/SR	161994	32640	40
Caelo	Wool alcohol cream DAB/SR	161989	32641	40
Caelo	Wool alcohol cream DAB/SR	163129	32848	40
Caelo	Wool alcohol cream DAB/SR	163131	32849	40
Caelo	Wool alcohol cream DAB/SR	162779	32850	40
Caelo	Wool alcohol cream DAB/SR	162782	32851	40
Caelo	Wool alcohol cream DAB/SR	162783	32852	40

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Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Wool alcohol cream DAB/SR	162781	32853	40
Caelo	Wool alcohol cream DAB/SR	162823	32854	40
Caelo	Wool alcohol cream DAB/SR	163130	32887	40

- 60 774 spectra from a total of 1424 batches from further 439 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.

- 1988 spectra from 252 *Apo-Ident* customers from 733 batches from the substance/substance group *Wool alcohol cream DAB/SR*.

Supplier	Substance	Batch	Spectra
Caelo	Wool alcohol cream DAB/SR	15360802	5
Caelo	Wool alcohol cream DAB/SR	13145201	7
Caelo	Wool alcohol cream DAB/SR	15361601	3
Caelo	Wool alcohol cream DAB/SR	15361501	4
Phoenix	Wool alcohol cream DAB/SR	16007701	1
Caelo	Wool alcohol cream DAB/SR	15361101	3
Caelo	Wool alcohol cream DAB/SR	16008103	13
Caelo	Wool alcohol cream DAB/SR	16007701	6
Caelo	Wool alcohol cream DAB/SR	16008301	4
Caelo	Wool alcohol cream DAB/SR	16008401	1
Caelo	Wool alcohol cream DAB/SR	16090301	2
Caesar & Loretz/Noweda	Wool alcohol cream DAB/SR	16008401	1
Caelo	Wool alcohol cream DAB/SR	16089902	4
Caelo	Wool alcohol cream DAB/SR	16090401	7
Caelo	Wool alcohol cream DAB/SR	16090101	1
Caelo	Wool alcohol cream DAB/SR	16090702	5
Caelo	Wool alcohol cream DAB/SR	16090501	12
Caelo	Wool alcohol cream DAB/SR	16157801	2
Caelo	Wool alcohol cream DAB/SR	16112201	2
Sanacorp/AHD	Wool alcohol cream DAB/SR	16157801	1
Caelo	Wool alcohol cream DAB/SR	16157802	5
Caelo	Wool alcohol cream DAB/SR	16157901	7
Caesar & Loretz GmbH Hi...	Wool alcohol cream DAB/SR	16157901	1
Caelo	Wool alcohol cream DAB/SR	16158001	3
Caelo	Wool alcohol cream DAB/SR	16158101	2
Caelo	Wool alcohol cream DAB/SR	16199004	1
Caelo	Wool alcohol cream DAB/SR	16199003	1
Caelo	Wool alcohol cream DAB/SR	16277902	4
Caelo	Wool alcohol cream DAB/SR	16277903	3
Caelo	Wool alcohol cream DAB/SR	16199201	1
Caelo	Wool alcohol cream DAB/SR	16340701	1
Caesar & Loretz/Noweda	Wool alcohol cream DAB/SR	16199401	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
Caelo	Wool alcohol cream DAB/SR	16282301	3
Caelo	Wool alcohol cream DAB/SR	2716Q-01371	1
Caelo	Wool alcohol cream DAB/SR	1015E-01371	1
Caelo	Wool alcohol cream DAB/SR	14259601	8
Caelo	Wool alcohol cream DAB/SR	14362501	5
Caelo	Wool alcohol cream DAB/SR	15017901	6
Caelo	Wool alcohol cream DAB/SR	14295601	5
Caelo	Wool alcohol cream DAB/SR	15017801	3
Caelo	Wool alcohol cream DAB/SR	15017601	10
Caelo	Wool alcohol cream DAB/SR	14259701	2
Caelo	Wool alcohol cream DAB/SR	15073601	11
Caelo	Wool alcohol cream DAB/SR	15073801	2
Caelo	Wool alcohol cream DAB/SR	15150002	2
Caelo	Wool alcohol cream DAB/SR	15149801	5
Caelo	Wool alcohol cream DAB/SR	15150101	5
Caelo	Wool alcohol cream DAB/SR	15226301	2
Caelo	Wool alcohol cream DAB/SR	15259701	12
Caelo	Wool alcohol cream DAB/SR	15259801	4
Caelo	Wool alcohol cream DAB/SR	15259802	1
Caelo	Wool alcohol cream DAB/SR	15260001	5
Caelo	Wool alcohol cream DAB/SR	15259901	3
Caelo	Wool alcohol cream DAB/SR	15260102	11
Caelo	Wool alcohol cream DAB/SR	15266001	4
Caelo	Wool alcohol cream DAB/SR	1526601	1
Caelo	Wool alcohol cream DAB/SR	15266101	1
Caelo	Wool alcohol cream DAB/SR	15266201	6
Caelo	Wool alcohol cream DAB/SR	15266301	3
Caesar&Loretz/Caesar&Lo...	Wool alcohol cream DAB/SR	15266301	1
Caelo	Wool alcohol cream DAB/SR	15266401	2
Caelo	Wool alcohol cream DAB/SR	15266501	5
unisan	Wool alcohol cream DAB/SR	15266501	1
Caelo	Wool alcohol cream DAB/SR	1529701	1
Caelo	Wool alcohol cream DAB/SR	15360901	10
Caelo	Wool alcohol cream DAB/SR	15360902	4
Caelo	Wool alcohol cream DAB/SR	15361001	2
Caelo	Wool alcohol cream DAB/SR	15361301	4
Caelo	Wool alcohol cream DAB/SR	15361402	7
Caelo	Wool alcohol cream DAB/SR	16007702	2
Caelo	Wool alcohol cream DAB/SR	153671601	1
Caelo	Wool alcohol cream DAB/SR	16007801	1
Noweda/ Caesar & Loretz...	Wool alcohol cream DAB/SR	16007901	1
Caelo	Wool alcohol cream DAB/SR	16007802	2
Caelo	Wool alcohol cream DAB/SR	16007901	5
Fagron	Wool alcohol cream DAB/SR	16007901	1
Fiebig	Wool alcohol cream DAB/SR	16008201	1
Caelo	Wool alcohol cream DAB/SR	16008201	2
Caelo	Wool alcohol cream DAB/SR	1608001	1
Sanacorp	Wool alcohol cream DAB/SR	27/AKD4	1
Bombastus	Wool alcohol cream DAB/SR	295460	2
Caelo	Wool alcohol cream DAB/SR	80616-10	1
Caelo	Wool alcohol cream DAB/SR	1118956	1
Caelo	Wool alcohol cream DAB/SR	614E1371	1
Caelo	Wool alcohol cream DAB/SR	9071301	1
Caelo	Wool alcohol cream DAB/SR	1098277	1
Caelo	Wool alcohol cream DAB/SR	11171501	1
Caelo	Wool alcohol cream DAB/SR	11228001	2
Caelo	Wool alcohol cream DAB/SR	11356101	3
Ichthyol-Gesellschaft	Wool alcohol cream DAB/SR	11288302	1
Caelo	Wool alcohol cream DAB/SR	11356301	1
Caelo	Wool alcohol cream DAB/SR	11356001	2

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Supplier	Substance	Batch	Spectra
Caelo	Wool alcohol cream DAB/SR	11356201	1
Caelo	Wool alcohol cream DAB/SR	12000201	2
Caelo	Wool alcohol cream DAB/SR	11356501	1
Caelo	Wool alcohol cream DAB/SR	12001101	3
Caelo	Wool alcohol cream DAB/SR	12001201	1
Caelo	Wool alcohol cream DAB/SR	12000301	1
Caelo	Wool alcohol cream DAB/SR	11356601	1
Caelo	Wool alcohol cream DAB/SR	12001301	1
Caelo	Wool alcohol cream DAB/SR	12030701	1
Caelo	Wool alcohol cream DAB/SR	12030601	2
Caelo	Wool alcohol cream DAB/SR	120307010	1
Caelo	Wool alcohol cream DAB/SR	12036501	5
Caelo	Wool alcohol cream DAB/SR	12036601	5
Caelo	Wool alcohol cream DAB/SR	12056301	1
Caelo	Wool alcohol cream DAB/SR	12056401	3
Caelo	Wool alcohol cream DAB/SR	12056202	1
ANZAG am 18.05.2012	Wool alcohol cream DAB/SR	12056402	1
Caelo	Wool alcohol cream DAB/SR	12106001	4
Caelo	Wool alcohol cream DAB/SR	12101304	1
Caelo	Wool alcohol cream DAB/SR	12106102	3
Devesa	Wool alcohol cream DAB/SR	12106601	1
Caelo	Wool alcohol cream DAB/SR	12106701	2
Caelo	Wool alcohol cream DAB/SR	12106601	1
Caelo	Wool alcohol cream DAB/SR	12106401	3
Caelo	Wool alcohol cream DAB/SR	1211901	1
Noweda	Wool alcohol cream DAB/SR	12121901	3
Caelo	Wool alcohol cream DAB/SR	12122001	5
Caelo	Wool alcohol cream DAB/SR	12122002	4
Gehe	Wool alcohol cream DAB/SR	12122001	1
Caelo	Wool alcohol cream DAB/SR	12122101	6
Caelo	Wool alcohol cream DAB/SR	1212202	1
Caelo	Wool alcohol cream DAB/SR	12122201	1
Caelo	Wool alcohol cream DAB/SR	12123501	6
Caelo	Wool alcohol cream DAB/SR	12205401	1
Anzag 04.12.12	Wool alcohol cream DAB/SR	12205402	1
Caelo	Wool alcohol cream DAB/SR	12205701	6
Caelo	Wool alcohol cream DAB/SR	12205501	1
Caelo	Wool alcohol cream DAB/SR	12205402	1
Caelo	Wool alcohol cream DAB/SR	12205801	3
Caelo	Wool alcohol cream DAB/SR	12208902	8
Noweda	Wool alcohol cream DAB/SR	12208902	1
Post-Apotheke	Wool alcohol cream DAB/SR	12209001	2
Caelo	Wool alcohol cream DAB/SR	12209001	2
anzag, 05.11.2012	Wool alcohol cream DAB/SR	12209101	1
Caelo	Wool alcohol cream DAB/SR	12209101	3
Caelo	Wool alcohol cream DAB/SR	12259701	3
Caelo	Wool alcohol cream DAB/SR	12259802	2
Caelo	Wool alcohol cream DAB/SR	12259702	4
Caelo	Wool alcohol cream DAB/SR	12260002	6
Caelo	Wool alcohol cream DAB/SR	12259901	3
Sanacorp	Wool alcohol cream DAB/SR	12260002	1
Caelo	Wool alcohol cream DAB/SR	12260101	2
Anzag 27.12.12 ek:9,46	Wool alcohol cream DAB/SR	12260101	1
Caelo	Wool alcohol cream DAB/SR	12260402	15
Caelo	Wool alcohol cream DAB/SR	12269201	4
Caelo	Wool alcohol cream DAB/SR	12307103	4
Caelo	Wool alcohol cream DAB/SR	12307102	1
phönix 22.01.2013	Wool alcohol cream DAB/SR	12307103	1
Caelo	Wool alcohol cream DAB/SR	12307201	8
Sanacorp	Wool alcohol cream DAB/SR	12307201	1

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Supplier	Substance	Batch	Spectra
Caelo	Wool alcohol cream DAB/SR	12307301	1
Caelo	Wool alcohol cream DAB/SR	12307501	4
Gehe	Wool alcohol cream DAB/SR	12307401	1
Caelo	Wool alcohol cream DAB/SR	12307401	6
Sanacorp	Wool alcohol cream DAB/SR	12307501	1
Großhandel	Wool alcohol cream DAB/SR	12307601	1
Caelo	Wool alcohol cream DAB/SR	12307601	5
Caelo	Wool alcohol cream DAB/SR	12307701	6
Caelo	Wool alcohol cream DAB/SR	12307801	2
Caelo	Wool alcohol cream DAB/SR	12307901	2
Caelo	Wool alcohol cream DAB/SR	12308001	6
Caelo	Wool alcohol cream DAB/SR	12370202	2
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	12307901	1
Fagron	Wool alcohol cream DAB/SR	12370202	1
Caelo	Wool alcohol cream DAB/SR	12351901	5
Phoenix 27.02.13	Wool alcohol cream DAB/SR	12308001	1
Caelo	Wool alcohol cream DAB/SR	12370401	11
Caelo	Wool alcohol cream DAB/SR	12370203	1
Großhandel	Wool alcohol cream DAB/SR	12370601	1
Caelo	Wool alcohol cream DAB/SR	12370601	9
Phoenix 11.03.13	Wool alcohol cream DAB/SR	1238001	1
Caelo	Wool alcohol cream DAB/SR	13029503	6
Finze	Wool alcohol cream DAB/SR	13029503	1
Caelo	Wool alcohol cream DAB/SR	13029502	3
AHD 09.04.2013	Wool alcohol cream DAB/SR	13029504	1
Caelo	Wool alcohol cream DAB/SR	13061401	3
Caelo	Wool alcohol cream DAB/SR	13061501	12
Caelo	Wool alcohol cream DAB/SR	13061402	3
Gehe	Wool alcohol cream DAB/SR	13061501	1
Caelo	Wool alcohol cream DAB/SR	13061601	4
gumo	Wool alcohol cream DAB/SR	13061701	2
Fagron	Wool alcohol cream DAB/SR	13061701	1
Caelo	Wool alcohol cream DAB/SR	13061901	7
Ichthyol/Phönix	Wool alcohol cream DAB/SR	13061801	2
Caelo	Wool alcohol cream DAB/SR	13062101	13
Post-Apotheke	Wool alcohol cream DAB/SR	13062001	1
Großhandel	Wool alcohol cream DAB/SR	13061901	1
Sanacorp	Wool alcohol cream DAB/SR	13062101	2
Gehe 02.07.2013	Wool alcohol cream DAB/SR	13062201	3
Caelo	Wool alcohol cream DAB/SR	13062201	3
Gehe	Wool alcohol cream DAB/SR	13062101	1
Caelo	Wool alcohol cream DAB/SR	13062301	5
Caelo	Wool alcohol cream DAB/SR	13068701	9
Caelo	Wool alcohol cream DAB/SR	13066501	1
Caelo/ Noweda	Wool alcohol cream DAB/SR	13068504	2
Caelo	Wool alcohol cream DAB/SR	13145202	6
Caesar & Loretz/ Noweda	Wool alcohol cream DAB/SR	13145202	1
Caelo	Wool alcohol cream DAB/SR	13145301	8
Caelo	Wool alcohol cream DAB/SR	13145501	4
A.H. 25.06.13 ek: 9,75EUR	Wool alcohol cream DAB/SR	13145501	1
Caelo	Wool alcohol cream DAB/SR	13145401	4
Caelo	Wool alcohol cream DAB/SR	13145601	11
Großhandel	Wool alcohol cream DAB/SR	13145501	1
Caelo	Wool alcohol cream DAB/SR	13145701	3
DEFEKTUR	Wool alcohol cream DAB/SR	13145801	1
Gehe 26.09.13	Wool alcohol cream DAB/SR	13146001	1
Anzag	Wool alcohol cream DAB/SR	13145801	2
Caesar & Loretz GmbH, 4. ...	Wool alcohol cream DAB/SR	13171901	1
Caelo	Wool alcohol cream DAB/SR	13145901	4
Caelo	Wool alcohol cream DAB/SR	13145801	7

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Supplier	Substance	Batch	Spectra
Caelo	Wool alcohol cream DAB/SR	13190201	1
Caelo	Wool alcohol cream DAB/SR	13146001	1
Caelo	Wool alcohol cream DAB/SR	13172103	11
Bombastus	Wool alcohol cream DAB/SR	13145901	1
Großhandel	Wool alcohol cream DAB/SR	13190203	1
Caelo	Wool alcohol cream DAB/SR	13261701	11
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	13261701	1
Caelo	Wool alcohol cream DAB/SR	13261801	10
Caelo	Wool alcohol cream DAB/SR	13279001	6
Caelo	Wool alcohol cream DAB/SR	13279101	4
Gehe 24.10.2013	Wool alcohol cream DAB/SR	13279002	1
Caelo	Wool alcohol cream DAB/SR	13279201	4
Caelo	Wool alcohol cream DAB/SR	13279002	2
Gehe	Wool alcohol cream DAB/SR	13279002	1
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	13279301	1
Phönix	Wool alcohol cream DAB/SR	13279301	1
Caelo	Wool alcohol cream DAB/SR	13279301	2
Caelo	Wool alcohol cream DAB/SR	13279502	4
Caelo	Wool alcohol cream DAB/SR	13279401	3
Caelo	Wool alcohol cream DAB/SR	13279701	2
Caelo	Wool alcohol cream DAB/SR	13289301	9
Fagron	Wool alcohol cream DAB/SR	13289301	1
Gehe am 03.02.2014	Wool alcohol cream DAB/SR	13289301	1
Caelo	Wool alcohol cream DAB/SR	13289403	6
Gehe am 14.01.2014	Wool alcohol cream DAB/SR	13289403	1
Noweda	Wool alcohol cream DAB/SR	13322801	1
Caelo	Wool alcohol cream DAB/SR	13322801	16
Caelo	Wool alcohol cream DAB/SR	13369401	5
Caelo	Wool alcohol cream DAB/SR	1336901	1
Caelo	Wool alcohol cream DAB/SR	13369601	11
Sanacorp	Wool alcohol cream DAB/SR	13369601	1
Alliance Health 07.01.2...	Wool alcohol cream DAB/SR	13369701	1
Caelo	Wool alcohol cream DAB/SR	13369701	4
Caelo	Wool alcohol cream DAB/SR	13369801	5
Caelo	Wool alcohol cream DAB/SR	13373501	2
Caelo	Wool alcohol cream DAB/SR	13373601	4
Caelo	Wool alcohol cream DAB/SR	13373701	9
Caelo	Wool alcohol cream DAB/SR	13394101	9
Caelo	Wool alcohol cream DAB/SR	14002801	11
Caelo	Wool alcohol cream DAB/SR	13394102	22
Noweda	Wool alcohol cream DAB/SR	14002801	2
Caelo	Wool alcohol cream DAB/SR	14045602	1
Caelo	Wool alcohol cream DAB/SR	14045702	3
Caelo	Wool alcohol cream DAB/SR	14046201	4
Caelo	Wool alcohol cream DAB/SR	14126801	12
Caelo	Wool alcohol cream DAB/SR	14162503	4
Caelo	Wool alcohol cream DAB/SR	14046401	5
Caelo	Wool alcohol cream DAB/SR	14166901	3
Caelo	Wool alcohol cream DAB/SR	14164201	15
Phoenix	Wool alcohol cream DAB/SR	14164201	1
Caelo	Wool alcohol cream DAB/SR	14167101	5
Caelo	Wool alcohol cream DAB/SR	14170801	3
Caelo	Wool alcohol cream DAB/SR	1426401	1
Caelo	Wool alcohol cream DAB/SR	14259801	7
Caelo	Wool alcohol cream DAB/SR	14295801	5
Phönix	Wool alcohol cream DAB/SR	15259701	2
Celo	Wool alcohol cream DAB/SR	16008301	1
Caelo	Wool alcohol cream DAB/SR	16090601	1
Caelo	Wool alcohol cream DAB/SR	1913Q-01371	1
DEFEKTUR	Wool alcohol cream DAB/SR	2013/08/14	1

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Supplier	Substance	Batch	Spectra
Caelo	Wool alcohol cream DAB/SR	1608992	1
Caelo	Wool alcohol cream DAB/SR		1
Caelo	Wool alcohol cream DAB/SR	2x13279201	1
Post-Apotheke	Wool alcohol cream DAB/SR	5113F-07109	1
Caelo	Wool alcohol cream DAB/SR	22/AKD52	1
Caelo	Wool alcohol cream DAB/SR	Ch12307102	1
Caelo	Wool alcohol cream DAB/SR	E-090413-3	1
Apomix	Wool alcohol cream DAB/SR	3A160113	1
Caelo	Wool alcohol cream DAB/SR	13373801	4
Caelo	Wool alcohol cream DAB/SR	14045801	10
Caelo	Wool alcohol cream DAB/SR	14246101	3
Caelo	Wool alcohol cream DAB/SR	14162502	7
Caelo	Wool alcohol cream DAB/SR	14246201	3
Caelo	Wool alcohol cream DAB/SR	14362201	9
Caelo	Wool alcohol cream DAB/SR	14295401	2
Bombastus	Wool alcohol cream DAB/SR	284582	1
Bombastus	Wool alcohol cream DAB/SR	287087	2
Bombastus	Wool alcohol cream DAB/SR	289384	1
Bombastus	Wool alcohol cream DAB/SR	291264	1
Bombastus	Wool alcohol cream DAB/SR	289489	1
Bombastus	Wool alcohol cream DAB/SR	289393	1
Caelo	Wool alcohol cream DAB/SR	13029504	1
Sanacorp	Wool alcohol cream DAB/SR	13145601	1
Caelo	Wool alcohol cream DAB/SR	1314570	1
Caelo	Wool alcohol cream DAB/SR	13279201-3433311180	1
Caelo	Wool alcohol cream DAB/SR	13369402	2
Caelo	Wool alcohol cream DAB/SR	13373903	2
Bombastus	Wool alcohol cream DAB/SR	275911	1
Bombastus	Wool alcohol cream DAB/SR	279875	2
Bombastus	Wool alcohol cream DAB/SR	280386	1
Bombastus	Wool alcohol cream DAB/SR	280390	2
Bombastus	Wool alcohol cream DAB/SR	278827	1
Caelo	Wool alcohol cream DAB/SR	14092502	7
Caelo	Wool alcohol cream DAB/SR	14167001	1
Caelo	Wool alcohol cream DAB/SR	15017501	2
Sanacorp	Wool alcohol cream DAB/SR	15017601	1
Caelo	Wool alcohol cream DAB/SR	15017502	4
Bombastus	Wool alcohol cream DAB/SR	60080302	2
Bombastus	Wool alcohol cream DAB/SR	269832	1
Caelo	Wool alcohol cream DAB/SR	1206202	1
Bombastus	Wool alcohol cream DAB/SR	267046	1
Anzag	Wool alcohol cream DAB/SR	12122201	1
Anzag	Wool alcohol cream DAB/SR	12269201	1
Anzag	Wool alcohol cream DAB/SR	13029503	1
Caelo	Wool alcohol cream DAB/SR	13171901	6
Caelo	Wool alcohol cream DAB/SR	13068601	8
Gehe	Wool alcohol cream DAB/SR	272253	1
Bombastus	Wool alcohol cream DAB/SR	272263	1
Bombastus	Wool alcohol cream DAB/SR	272259	2
Bombastus	Wool alcohol cream DAB/SR	273631	2
Bombastus	Wool alcohol cream DAB/SR	277208	1
Gehe	Wool alcohol cream DAB/SR	277207	1
Gehe	Wool alcohol cream DAB/SR	282245	1
Bombastus	Wool alcohol cream DAB/SR	285875	1
Bombastus	Wool alcohol cream DAB/SR	284447	1
Gehe	Wool alcohol cream DAB/SR	288442	2
Caelo	Wool alcohol cream DAB/SR	1071503	1
apomix PKH GmbH Halle	Wool alcohol cream DAB/SR	6A220115	1
Apomix	Wool alcohol cream DAB/SR	1A020114	1
apomix/GEHE23.04.14	Wool alcohol cream DAB/SR	5A200114	1

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Supplier	Substance	Batch	Spectra
Apomix/Phönix	Wool alcohol cream DAB/SR	5A220115	1
Caelo	Wool alcohol cream DAB/SR	415A-01371	1
Gehe/Apomix	Wool alcohol cream DAB/SR	8A290114	1
Caelo	Wool alcohol cream DAB/SR	9041402	1
Apomix / Phönix	Wool alcohol cream DAB/SR	101A191213	1
apomix/Gehe	Wool alcohol cream DAB/SR	104A111214	1
Apomix	Wool alcohol cream DAB/SR	100A021214	1
Apomix/Gehe	Wool alcohol cream DAB/SR	104A091215	1
Pharmachem/Phönix	Wool alcohol cream DAB/SR	110614	1
Apomix/Noweda	Wool alcohol cream DAB/SR	105A301214	1
Apomix	Wool alcohol cream DAB/SR	108A301214	1
Pharmachem.Pößneck/Phoe...	Wool alcohol cream DAB/SR	110913	1
Pharmachem GmbH	Wool alcohol cream DAB/SR	110913	1
Caelo	Wool alcohol cream DAB/SR	114163901	1
Apomix/Noweda	Wool alcohol cream DAB/SR	12A040214	1
Caelo	Wool alcohol cream DAB/SR	13013201	1
Apomix/Noweda	Wool alcohol cream DAB/SR	12A050215	1
Caelo	Wool alcohol cream DAB/SR	13172102	1
Sanacorp	Wool alcohol cream DAB/SR	13172102	1
Caelo	Wool alcohol cream DAB/SR	13272601	1
Caelo	Wool alcohol cream DAB/SR	13280701	4
Caelo	Wool alcohol cream DAB/SR	13281003	4
Caelo	Wool alcohol cream DAB/SR	13369501	2
Großhandel	Wool alcohol cream DAB/SR	13373501	1
GEHE 24.02.2014	Wool alcohol cream DAB/SR	13373801	1
Caesar & Loretz GmbH Hi...	Wool alcohol cream DAB/SR	13373701	1
Caelo	Wool alcohol cream DAB/SR	13394103	2
Caelo	Wool alcohol cream DAB/SR	13394201	5
Gehe	Wool alcohol cream DAB/SR	13394201	1
Apomix	Wool alcohol cream DAB/SR	13A050215	1
Caelo	Wool alcohol cream DAB/SR	14033202	3
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	14045702	1
Ichthyol Gesellschaft	Wool alcohol cream DAB/SR	14045801	1
Caelo	Wool alcohol cream DAB/SR	14045901	4
Caelo	Wool alcohol cream DAB/SR	14046101	2
Caelo	Wool alcohol cream DAB/SR	14046001	1
Phönix	Wool alcohol cream DAB/SR	14046101	1
Caelo	Wool alcohol cream DAB/SR	14046002	1
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	14046201	1
Sanacorp	Wool alcohol cream DAB/SR	14046401	1
Caelo	Wool alcohol cream DAB/SR	14046501	4
Caelo	Wool alcohol cream DAB/SR	14046502	2
Caelo	Wool alcohol cream DAB/SR	14092401	3
Caelo	Wool alcohol cream DAB/SR	14092501	16
Caelo	Wool alcohol cream DAB/SR	14092601	5
Sana	Wool alcohol cream DAB/SR	14092502	1
Caelo	Wool alcohol cream DAB/SR	14113201	4
Phönix	Wool alcohol cream DAB/SR	14162502	1
Caelo	Wool alcohol cream DAB/SR	14164001	2
Caelo	Wool alcohol cream DAB/SR	14164101	1
Caelo	Wool alcohol cream DAB/SR	14163901	1
Sanacorp	Wool alcohol cream DAB/SR	14164101	1
Phönix	Wool alcohol cream DAB/SR	14164201	2
Fagron	Wool alcohol cream DAB/SR	14164201	1
Caelo	Wool alcohol cream DAB/SR	14169101	8
Phönix	Wool alcohol cream DAB/SR	14169101	3
Caelo	Wool alcohol cream DAB/SR	14169201	4
Caelo	Wool alcohol cream DAB/SR	14170901	1
Euro OTC	Wool alcohol cream DAB/SR	14170901	1
Caelo	Wool alcohol cream DAB/SR	14216601	5

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Supplier	Substance	Batch	Spectra
Phönix	Wool alcohol cream DAB/SR	14170801	1
Caelo	Wool alcohol cream DAB/SR	14216701	2
Caelo	Wool alcohol cream DAB/SR	14216801	5
Caelo	Wool alcohol cream DAB/SR	14216901	2
Caelo	Wool alcohol cream DAB/SR	14216902	12
Fagron	Wool alcohol cream DAB/SR	14216902	1
Caelo	Wool alcohol cream DAB/SR	14216903	2
Caelo	Wool alcohol cream DAB/SR	14246301	3
Caelo	Wool alcohol cream DAB/SR	14246102	1
Phönix	Wool alcohol cream DAB/SR	14246301	1
Caelo	Wool alcohol cream DAB/SR	14246401	6
Gehe	Wool alcohol cream DAB/SR	14246401	1
Caelo	Wool alcohol cream DAB/SR	14246501	5
Ichthyol	Wool alcohol cream DAB/SR	14246501	1
Caelo	Wool alcohol cream DAB/SR	14259401	5
Caelo	Wool alcohol cream DAB/SR	14259402	1
Caelo	Wool alcohol cream DAB/SR	14259501	1
Caelo	Wool alcohol cream DAB/SR	14295301	2
Caelo	Wool alcohol cream DAB/SR	1429501	1
Noweda	Wool alcohol cream DAB/SR	14295402	1
Caelo	Wool alcohol cream DAB/SR	14295502	4
Caelo	Wool alcohol cream DAB/SR	14295402	1
Alliance10.02.2015	Wool alcohol cream DAB/SR	14295502	2
Caelo	Wool alcohol cream DAB/SR	14295701	3
Sanacorp	Wool alcohol cream DAB/SR	14295701	1
Caelo	Wool alcohol cream DAB/SR	14295901	3
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	14295901	1
Caelo	Wool alcohol cream DAB/SR	14296001	5
Caelo	Wool alcohol cream DAB/SR	14356301	2
Caelo	Wool alcohol cream DAB/SR	14356302	15
Bombastus	Wool alcohol cream DAB/SR	14356302	5
Caelo	Wool alcohol cream DAB/SR	14356401	1
Caelo	Wool alcohol cream DAB/SR	14356402	4
Caelo	Wool alcohol cream DAB/SR	14356501	1
Phönix	Wool alcohol cream DAB/SR	14362102	1
Caelo	Wool alcohol cream DAB/SR	14356601	1
Caelo	Wool alcohol cream DAB/SR	14362102	3
Caelo	Wool alcohol cream DAB/SR	1436201	1
Alliance Health 06.03.2...	Wool alcohol cream DAB/SR	14362102	1
Caelo	Wool alcohol cream DAB/SR	14362301	3
Caelo	Wool alcohol cream DAB/SR	14362401	2
Allianz Healthcare 27.0...	Wool alcohol cream DAB/SR	14362401	2
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	14362301	1
Phoenix	Wool alcohol cream DAB/SR	14362501	2
Apomix/Sana	Wool alcohol cream DAB/SR	14A180215	3
Caelo	Wool alcohol cream DAB/SR	15011504	1
Caelo	Wool alcohol cream DAB/SR	15017701	2
Phoenix Goettin	Wool alcohol cream DAB/SR	15017801	1
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	15017801	1
Caelo	Wool alcohol cream DAB/SR	15022201	3
Caelo	Wool alcohol cream DAB/SR	15073502	1
Caelo	Wool alcohol cream DAB/SR	15073301	1
Fagron	Wool alcohol cream DAB/SR	15073701	1
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	15073701	1
Caelo	Wool alcohol cream DAB/SR	151110	1
Caelo	Wool alcohol cream DAB/SR	15132101	8
Caelo	Wool alcohol cream DAB/SR	15150001	3
Caelo	Wool alcohol cream DAB/SR	15132301	2
Caelo	Wool alcohol cream DAB/SR	15149902	1
Caelo	Wool alcohol cream DAB/SR	15174103	3

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Supplier	Substance	Batch	Spectra
Caelo	Wool alcohol cream DAB/SR	15174104	11
Caelo	Wool alcohol cream DAB/SR	15174201	5
Caelo	Wool alcohol cream DAB/SR	15174105	1
Caelo	Wool alcohol cream DAB/SR	15174301	3
Caelo	Wool alcohol cream DAB/SR	15174302	3
Phönix Gotha	Wool alcohol cream DAB/SR	151831	1
Leyh Pharma GmbH	Wool alcohol cream DAB/SR	151831	1
Caelo	Wool alcohol cream DAB/SR	15268302	11
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	15266501	1
Caelo	Wool alcohol cream DAB/SR	15268/601	1
Anzag	Wool alcohol cream DAB/SR	15268302	1
Caelo	Wool alcohol cream DAB/SR	15268303	1
Celo/ Noweda	Wool alcohol cream DAB/SR	15268401	2
Caelo	Wool alcohol cream DAB/SR	15268601	9
Caelo	Wool alcohol cream DAB/SR	15268401	1
Caelo	Wool alcohol cream DAB/SR	15268501	3
Noweda	Wool alcohol cream DAB/SR	15268601	1
Caelo	Wool alcohol cream DAB/SR	15360801	1
Caelo	Wool alcohol cream DAB/SR	15361201	1
Caelo	Wool alcohol cream DAB/SR	15361701	1
Apomix/Gehe	Wool alcohol cream DAB/SR	15A230215	1
Caelo	Wool alcohol cream DAB/SR	16024401	3
Caelo	Wool alcohol cream DAB/SR	16024301	1
Noweda	Wool alcohol cream DAB/SR	16024403	1
Caelo	Wool alcohol cream DAB/SR	16024501	2
Phoenix	Wool alcohol cream DAB/SR	16024501	1
Caelo	Wool alcohol cream DAB/SR	16024403	1
Noweda	Wool alcohol cream DAB/SR	16024601	1
Caelo	Wool alcohol cream DAB/SR	161177701	1
Caelo	Wool alcohol cream DAB/SR	16120802	1
Caelo	Wool alcohol cream DAB/SR	16177401	3
Gehe	Wool alcohol cream DAB/SR	16177401	2
PHÖNIX	Wool alcohol cream DAB/SR	16177502	1
Caelo	Wool alcohol cream DAB/SR	16177602	1
Phoenix	Wool alcohol cream DAB/SR	16177701	1
Caelo	Wool alcohol cream DAB/SR	16177701	2
Caelo	Wool alcohol cream DAB/SR	16177601	1
Apomix/Noweda	Wool alcohol cream DAB/SR	17A230215	1
Apomix/Noweda	Wool alcohol cream DAB/SR	20A270214	1
Apomix / Phönix	Wool alcohol cream DAB/SR	21A280214	2
Gehe/Apomix	Wool alcohol cream DAB/SR	19A270214	1
Sanacorp	Wool alcohol cream DAB/SR	22/AKD2	1
Euro OTC	Wool alcohol cream DAB/SR	221014	1
Sanacorp	Wool alcohol cream DAB/SR	25/AKD3	1
Caelo	Wool alcohol cream DAB/SR	23101405	1
Bombastus	Wool alcohol cream DAB/SR	274683	2
Bombastus	Wool alcohol cream DAB/SR	277856	3
Bombastus	Wool alcohol cream DAB/SR	279021	1
Bombastus	Wool alcohol cream DAB/SR	279019	2
Bombastus	Wool alcohol cream DAB/SR	28/7175	1
Bombastus	Wool alcohol cream DAB/SR	280391	1
Bombastus	Wool alcohol cream DAB/SR	281503	2
Bombastus	Wool alcohol cream DAB/SR	280988	1
Bombastus	Wool alcohol cream DAB/SR	282751	3
Bombastus	Wool alcohol cream DAB/SR	282753	2
Bombastus	Wool alcohol cream DAB/SR	283574	1
Bombastus	Wool alcohol cream DAB/SR	284450	1
Bombastus	Wool alcohol cream DAB/SR	284577	1
Bombastus	Wool alcohol cream DAB/SR	284579	4
Bombastus	Wool alcohol cream DAB/SR	284580	1

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Supplier	Substance	Batch	Spectra
Bombastus	Wool alcohol cream DAB/SR	284636	3
Bombastus	Wool alcohol cream DAB/SR	284638	1
Bombastus	Wool alcohol cream DAB/SR	284943	1
Bombastus	Wool alcohol cream DAB/SR	284951	2
Bombastus	Wool alcohol cream DAB/SR	285109	1
Bombastus	Wool alcohol cream DAB/SR	285867	1
Bombastus	Wool alcohol cream DAB/SR	285817	1
gehe	Wool alcohol cream DAB/SR	285868	1
GEHE/B0mbastus/04.14	Wool alcohol cream DAB/SR	285870	1
Bombastus	Wool alcohol cream DAB/SR	285868	1
Bombastus	Wool alcohol cream DAB/SR	285874	1
Bombastus	Wool alcohol cream DAB/SR	285869	1
Gehe	Wool alcohol cream DAB/SR	285873	1
Bombastus	Wool alcohol cream DAB/SR	285872	2
Bombastus	Wool alcohol cream DAB/SR	286234	1
Bombastus	Wool alcohol cream DAB/SR	286233	1
Bombastus	Wool alcohol cream DAB/SR	286236	2
Bombastus	Wool alcohol cream DAB/SR	286237	1
Bombastus	Wool alcohol cream DAB/SR	286238	1
Bombastus	Wool alcohol cream DAB/SR	287085	1
Bombastus	Wool alcohol cream DAB/SR	287093	3
Bombastus	Wool alcohol cream DAB/SR	287179	2
Bombastus	Wool alcohol cream DAB/SR	287176	1
Gehe 21.08.14	Wool alcohol cream DAB/SR	287175	1
Bombastus	Wool alcohol cream DAB/SR	288259	2
Bombastus	Wool alcohol cream DAB/SR	288260	1
Bombastus	Wool alcohol cream DAB/SR	288261	1
Bombastus	Wool alcohol cream DAB/SR	288351	1
Bombastus	Wool alcohol cream DAB/SR	288355	2
Bombastus	Wool alcohol cream DAB/SR	288442	1
Bombastus	Wool alcohol cream DAB/SR	288441	1
Bombastus	Wool alcohol cream DAB/SR	288443	5
Bombastus	Wool alcohol cream DAB/SR	288446	3
Bombastus	Wool alcohol cream DAB/SR	289088	1
Bombastus	Wool alcohol cream DAB/SR	289091	2
Bombastus	Wool alcohol cream DAB/SR	289394	1
Bombastus	Wool alcohol cream DAB/SR	289390	1
Bombastus	Wool alcohol cream DAB/SR	289487	2
Bombastus	Wool alcohol cream DAB/SR	289391	1
Bombastus	Wool alcohol cream DAB/SR	289395	1
Bombastus	Wool alcohol cream DAB/SR	289396	1
Bombastus	Wool alcohol cream DAB/SR	289490	1
Bombastus	Wool alcohol cream DAB/SR	291265	1
Bombastus	Wool alcohol cream DAB/SR	291267	1
Bombastus	Wool alcohol cream DAB/SR	291272	1
Bombastus	Wool alcohol cream DAB/SR	291348	2
Bombastus	Wool alcohol cream DAB/SR	291352	3
Bombastus	Wool alcohol cream DAB/SR	291433	1
Bombastus	Wool alcohol cream DAB/SR	291477	1
Bombastus	Wool alcohol cream DAB/SR	292769	1
Bombastus	Wool alcohol cream DAB/SR	292693	1
Bombastus	Wool alcohol cream DAB/SR	292695	2
Bombastus	Wool alcohol cream DAB/SR	293069	2
Bombastus	Wool alcohol cream DAB/SR	294270	2
Bombastus	Wool alcohol cream DAB/SR	294272	3
Bombastus	Wool alcohol cream DAB/SR	294271	2
Bombastus	Wool alcohol cream DAB/SR	294273	1
Bombastus	Wool alcohol cream DAB/SR	294527	1
Bombastus	Wool alcohol cream DAB/SR	294529	1
Bombastus	Wool alcohol cream DAB/SR	295218	1

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Supplier	Substance	Batch	Spectra
Bombastus	Wool alcohol cream DAB/SR	294533	1
Bombastus	Wool alcohol cream DAB/SR	295462	2
Bombastus	Wool alcohol cream DAB/SR	295464	1
Bombastus	Wool alcohol cream DAB/SR	295528	1
Bombastus	Wool alcohol cream DAB/SR	295529	3
Bombastus	Wool alcohol cream DAB/SR	295532	1
Bombastus	Wool alcohol cream DAB/SR	295534	1
Bombastus	Wool alcohol cream DAB/SR	295536	4
Bombastus	Wool alcohol cream DAB/SR	296133	1
Caelo	Wool alcohol cream DAB/SR	296128	1
Bombastus	Wool alcohol cream DAB/SR	296128	1
Caelo	Wool alcohol cream DAB/SR	296131	2
Bombastus	Wool alcohol cream DAB/SR	297526	1
Bombastus	Wool alcohol cream DAB/SR	297527	2
Bombastus	Wool alcohol cream DAB/SR	297529	4
Bombastus	Wool alcohol cream DAB/SR	297528	1
Bombastus	Wool alcohol cream DAB/SR	297531	5
Bombastus	Wool alcohol cream DAB/SR	297530	1
Bombastus	Wool alcohol cream DAB/SR	298675	2
Bombastus	Wool alcohol cream DAB/SR	298678	2
Bombastus	Wool alcohol cream DAB/SR	298679	1
Bombastus	Wool alcohol cream DAB/SR	298814	1
Bombastus	Wool alcohol cream DAB/SR	298815	2
Bombastus	Wool alcohol cream DAB/SR	298816	3
Bombastus	Wool alcohol cream DAB/SR	299227	1
Bombastus	Wool alcohol cream DAB/SR	299231	3
Bombastus	Wool alcohol cream DAB/SR	299233	1
Bombastus	Wool alcohol cream DAB/SR	299234	4
Bombastus	Wool alcohol cream DAB/SR	299232	1
Bombastus	Wool alcohol cream DAB/SR	299785	1
Bombastus	Wool alcohol cream DAB/SR	299784	1
Bombastus	Wool alcohol cream DAB/SR	299782	1
Bombastus	Wool alcohol cream DAB/SR	300577	3
Bombastus	Wool alcohol cream DAB/SR	300579	2
Bombastus	Wool alcohol cream DAB/SR	300581	2
Phoenix	Wool alcohol cream DAB/SR	300583	1
Bombastus	Wool alcohol cream DAB/SR	300831	1
Bombastus	Wool alcohol cream DAB/SR	300833	1
Bombastus	Wool alcohol cream DAB/SR	300836	1
Bombastus	Wool alcohol cream DAB/SR	300837	1
Bombastus	Wool alcohol cream DAB/SR	301308	2
Bombastus	Wool alcohol cream DAB/SR	301310	2
Bombastus	Wool alcohol cream DAB/SR	301309	1
Bombastus	Wool alcohol cream DAB/SR	301312	1
Phönix	Wool alcohol cream DAB/SR	301312	1
Bombastus	Wool alcohol cream DAB/SR	301889	1
Bombastus	Wool alcohol cream DAB/SR	301885	1
Bombastus	Wool alcohol cream DAB/SR	301891	1
Bombastus	Wool alcohol cream DAB/SR	302032	2
Bombastus	Wool alcohol cream DAB/SR	302030	1
Bombastus	Wool alcohol cream DAB/SR	302031	2
Bombastus	Wool alcohol cream DAB/SR	302966	4
Bombastus	Wool alcohol cream DAB/SR	302968	1
Bombastus	Wool alcohol cream DAB/SR	302969	1
Bombastus	Wool alcohol cream DAB/SR	302970	1
Caelo	Wool alcohol cream DAB/SR	303524	1
Bombastus	Wool alcohol cream DAB/SR	304429	2
Bombastus	Wool alcohol cream DAB/SR	304428	1
Bombastus	Wool alcohol cream DAB/SR	304436	1
apomix PKH GmbH Halle	Wool alcohol cream DAB/SR	32A120416	1

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Supplier	Substance	Batch	Spectra
Bombastus	Wool alcohol cream DAB/SR	305257	1
Bombastus	Wool alcohol cream DAB/SR	304437	1
apomix/Noweda	Wool alcohol cream DAB/SR	31A110416	1
Apomix	Wool alcohol cream DAB/SR	32A120416	1
Apomix / Phönix	Wool alcohol cream DAB/SR	33A010414	1
apomix/Holdermann	Wool alcohol cream DAB/SR	34A250516	2
apomix	Wool alcohol cream DAB/SR	34A250516	1
Apomix/Gehe	Wool alcohol cream DAB/SR	37A220415	2
Apomix/Noweda	Wool alcohol cream DAB/SR	37A090414	1
Caelo	Wool alcohol cream DAB/SR	37A090414	1
Raben-Apotheke Mildenau	Wool alcohol cream DAB/SR	38A150514	1
apomix/Phönix	Wool alcohol cream DAB/SR	39A050716	1
Euro OTC	Wool alcohol cream DAB/SR	39A150514	1
Bombastus	Wool alcohol cream DAB/SR	40/14	1
PKH GmbH	Wool alcohol cream DAB/SR	40A080816	1
Apomix PKH GmbH	Wool alcohol cream DAB/SR	40A080816	1
apomix PKH GmbH Halle	Wool alcohol cream DAB/SR	41A230415	1
Euro OTC	Wool alcohol cream DAB/SR	43A041016	1
Phönix	Wool alcohol cream DAB/SR		1
apomix/Phönix	Wool alcohol cream DAB/SR	43A200515	1
Raben-Apotheke Mildenau	Wool alcohol cream DAB/SR	45A260514	3
apomix PKH GmbH Halle	Wool alcohol cream DAB/SR	46A27515	1
Bombastus	Wool alcohol cream DAB/SR	47/14	1
Gehe/20.08.14/Apomix	Wool alcohol cream DAB/SR	48A110614	1
Apomix / Phönix	Wool alcohol cream DAB/SR	48A110614	1
Apomix/Gehe	Wool alcohol cream DAB/SR	50A110614	1
apomix	Wool alcohol cream DAB/SR	58A100615	1
Apomix/Phoenix	Wool alcohol cream DAB/SR	56A300614	1
PKH GmbH,Phönix	Wool alcohol cream DAB/SR	57A100615	1
Lamotte/Noweda	Wool alcohol cream DAB/SR	553700	1
Apomix / Phoenix	Wool alcohol cream DAB/SR	57A100615	1
apomix PKH GmbH Halle	Wool alcohol cream DAB/SR	57A300614	1
Apomix	Wool alcohol cream DAB/SR	61A080714	2
Apomix/Noweda	Wool alcohol cream DAB/SR	62A250615	1
Gehe/apomix/23.09.14	Wool alcohol cream DAB/SR	62A090714	1
apomix/Holdermann	Wool alcohol cream DAB/SR	62A090714	1
apomix PKH GmbH Halle	Wool alcohol cream DAB/SR	69A120815	1
Apomix	Wool alcohol cream DAB/SR	64A250715	1
Apomix/Alliance Healthc. . .	Wool alcohol cream DAB/SR	66A060715	1
apomix PKH GmbH Halle	Wool alcohol cream DAB/SR	72-A190814	1
apomix/Phönix	Wool alcohol cream DAB/SR	74A130815	1
Apomix	Wool alcohol cream DAB/SR	74A130815	1
apomix/Holdermann	Wool alcohol cream DAB/SR	78A160913	1
Apomix/Noweda	Wool alcohol cream DAB/SR	77A260815	1
apomix/Noweda	Wool alcohol cream DAB/SR	75A130815	1
Taoasis	Wool alcohol cream DAB/SR	81/12	1
GEHE/Apomix/31.01.14	Wool alcohol cream DAB/SR	82A260913	1
Apomix/Noweda	Wool alcohol cream DAB/SR	81A290914	1
Apomix / Phönix	Wool alcohol cream DAB/SR	85A300914	1
Apomix	Wool alcohol cream DAB/SR	83A290914	2
Apomix/Gehe	Wool alcohol cream DAB/SR	87A061015	1
Apomix	Wool alcohol cream DAB/SR	85A300914	1
Gehe/apomix/17.12.2014	Wool alcohol cream DAB/SR	87A141014	1
Apomix/Sana	Wool alcohol cream DAB/SR	89A291015	1
apomix PKH GmbH Halle	Wool alcohol cream DAB/SR	89A291015	1
apomix/Noweda	Wool alcohol cream DAB/SR	90A221014	1
Apomix/Sana	Wool alcohol cream DAB/SR	90A291015	1
Apomix	Wool alcohol cream DAB/SR	92A281014	1
Apomix	Wool alcohol cream DAB/SR	96A181114	4
Apomix	Wool alcohol cream DAB/SR	92A111115	1

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Supplier	Substance	Batch	Spectra
apomix/Holdermann	Wool alcohol cream DAB/SR	93A111115	1
Bombastus	Wool alcohol cream DAB/SR	256922	1
Bombastus	Wool alcohol cream DAB/SR	265187	1
Bombastus	Wool alcohol cream DAB/SR	267043	1
Bombastus	Wool alcohol cream DAB/SR	267154	1
Gehe	Wool alcohol cream DAB/SR	267155	2
Bombastus	Wool alcohol cream DAB/SR	268902	1
Bombastus	Wool alcohol cream DAB/SR	269927	1
Gehe	Wool alcohol cream DAB/SR	269933	2
Bombastus	Wool alcohol cream DAB/SR	269924	1
Gehe	Wool alcohol cream DAB/SR	270032	1
Bombastus	Wool alcohol cream DAB/SR	270033	2
Gehe	Wool alcohol cream DAB/SR	270037	1
Bombastus	Wool alcohol cream DAB/SR	270038	1
Bombastus	Wool alcohol cream DAB/SR	270629	1
Gehe	Wool alcohol cream DAB/SR	270720	1
Bombastus	Wool alcohol cream DAB/SR	270725	2
Bombastus	Wool alcohol cream DAB/SR	271811	1
Bombastus	Wool alcohol cream DAB/SR	271812	1
Gehe	Wool alcohol cream DAB/SR	272254	1
Bombastus	Wool alcohol cream DAB/SR	272254	1
Bombastus	Wool alcohol cream DAB/SR	273637	1
Bombastus	Wool alcohol cream DAB/SR	272257	1
Bombastus	Wool alcohol cream DAB/SR	273634	1
Caelo	Wool alcohol cream DAB/SR	273635	1
Bombastus	Wool alcohol cream DAB/SR	274347	1
Noweda/apomix	Wool alcohol cream DAB/SR	5A290113	2
Gehe/PKH	Wool alcohol cream DAB/SR	3A160113	1
Pharmachem.	Wool alcohol cream DAB/SR	81111	1
Caelo	Wool alcohol cream DAB/SR	9011407	1
Apomix	Wool alcohol cream DAB/SR	101A291012	1
Apomix	Wool alcohol cream DAB/SR	101A191213	1
Apomix	Wool alcohol cream DAB/SR	103A291012	3
Gehe	Wool alcohol cream DAB/SR	103A291012	1
Apomix	Wool alcohol cream DAB/SR	104A291012	1
apomix/GEHE/04.04.2013	Wool alcohol cream DAB/SR	108A191112	1
Apomix	Wool alcohol cream DAB/SR	109A191112	1
Caelo	Wool alcohol cream DAB/SR	1113E-01371	1
Caelo	Wool alcohol cream DAB/SR	1117601	1
Caelo	Wool alcohol cream DAB/SR	11226401	2
Caelo	Wool alcohol cream DAB/SR	11226201	1
Caelo	Wool alcohol cream DAB/SR	11226301	1
Caesar & Loretz GmbH, 4...	Wool alcohol cream DAB/SR	11276102	2
Gehe	Wool alcohol cream DAB/SR	11276102	2
Phönix Gotha	Wool alcohol cream DAB/SR	11226301	1
Anzag	Wool alcohol cream DAB/SR	11226402	1
Caelo	Wool alcohol cream DAB/SR	11276102	1
Caesar & Loretz GmbH, 4...	Wool alcohol cream DAB/SR	12000201	1
Caelo	Wool alcohol cream DAB/SR	115A171212	1
Caelo	Wool alcohol cream DAB/SR	12036401	2
Caelo	Wool alcohol cream DAB/SR	12036301	2
Caelo	Wool alcohol cream DAB/SR	12036402	3
Caelo	Wool alcohol cream DAB/SR	12036403	1
Phönix Gotha	Wool alcohol cream DAB/SR	12036403	1
Gehe	Wool alcohol cream DAB/SR	12036501	1
Caesar & Loretz GmbH, 4...	Wool alcohol cream DAB/SR	12036501	1
anzag	Wool alcohol cream DAB/SR	12036601	1
Caelo	Wool alcohol cream DAB/SR	12056402	1
Caelo	Wool alcohol cream DAB/SR	12101602	1
Caelo	Wool alcohol cream DAB/SR	12121901	1

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Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH, 4...	Wool alcohol cream DAB/SR	12123501	1
Anzag, 19.11.2012	Wool alcohol cream DAB/SR	12205601	1
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	12209101	1
Caelo	Wool alcohol cream DAB/SR	12260401	1
Anzag 28.03.2013	Wool alcohol cream DAB/SR	12260402	1
Caelo	Wool alcohol cream DAB/SR	1226901	1
Anzag 21.11.12	Wool alcohol cream DAB/SR	12269201	1
Caelo	Wool alcohol cream DAB/SR	1230401	1
Noweda	Wool alcohol cream DAB/SR	12307201	1
Krieger	Wool alcohol cream DAB/SR	12307601	1
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	12307801	1
Noweda	Wool alcohol cream DAB/SR	12308001	1
Caelo	Wool alcohol cream DAB/SR	12351801	1
Caelo	Wool alcohol cream DAB/SR	12352001	2
Phönix Gotha	Wool alcohol cream DAB/SR	12352001	1
12370401	Wool alcohol cream DAB/SR	12370401	1
Caesar & Loretz GmbH, 4...	Wool alcohol cream DAB/SR	12352001	1
Caelo	Wool alcohol cream DAB/SR	13008203	1
Caelo	Wool alcohol cream DAB/SR	13013202	8
Post-Apotheke	Wool alcohol cream DAB/SR	13013202	1
Caesar&loretz,Phoenix	Wool alcohol cream DAB/SR	13013202	1
Caelo	Wool alcohol cream DAB/SR	13061801	1
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	13061901	1
Phönix Gotha	Wool alcohol cream DAB/SR	13062101	1
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	13062201	1
Phönix	Wool alcohol cream DAB/SR	13062301	1
Caelo	Wool alcohol cream DAB/SR	13068501	4
Caelo	Wool alcohol cream DAB/SR	1306804	1
Caelo	Wool alcohol cream DAB/SR	13068503	3
Caesar&loretz,Phoenix	Wool alcohol cream DAB/SR	13068504	1
Alliance healthcare	Wool alcohol cream DAB/SR	13068504	6
Caelo	Wool alcohol cream DAB/SR	13068504	7
Phoenix	Wool alcohol cream DAB/SR	13068601	1
Fagron	Wool alcohol cream DAB/SR	13068601	1
Caelo	Wool alcohol cream DAB/SR	13081303	1
Gehe	Wool alcohol cream DAB/SR	13145801	1
Euro OTC	Wool alcohol cream DAB/SR	13145801	1
Caelo	Wool alcohol cream DAB/SR	13172001	7
Phönix Gotha	Wool alcohol cream DAB/SR	13172001	1
Caelo	Wool alcohol cream DAB/SR	13172104	1
Caesar&loretz,Phoenix	Wool alcohol cream DAB/SR	13172103	1
Caelo	Wool alcohol cream DAB/SR	13172105	2
Caelo	Wool alcohol cream DAB/SR	13190202	1
Caelo	Wool alcohol cream DAB/SR	13279601	2
Caelo	Wool alcohol cream DAB/SR	13280601	1
Caelo	Wool alcohol cream DAB/SR	13280801	2
PHOENIX 21.02.2014	Wool alcohol cream DAB/SR	13369402	1
Caesar & Loretz GmbH	Wool alcohol cream DAB/SR	13373601	1
Pöfneck Pharmachem	Wool alcohol cream DAB/SR	140312	1
Caelo	Wool alcohol cream DAB/SR	14031602	1
Caesar&loretz,Phoenix	Wool alcohol cream DAB/SR	14092501	2
Caesar&loretz,Phoenix	Wool alcohol cream DAB/SR	14200702	1
Caelo	Wool alcohol cream DAB/SR	1424501	1
Phoenix	Wool alcohol cream DAB/SR	14A180214	1
P.W.Beyvers GmbH,Phönix	Wool alcohol cream DAB/SR	15A230215	1
Apomix	Wool alcohol cream DAB/SR	19A120213	1
Caelo	Wool alcohol cream DAB/SR	20101112-1	1
Apomix	Wool alcohol cream DAB/SR	20A070212	1
Apomix	Wool alcohol cream DAB/SR	20A120213	1
Caelo	Wool alcohol cream DAB/SR	2112217035	1

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Supplier	Substance	Batch	Spectra
Apomix	Wool alcohol cream DAB/SR	21A070212	1
apomix	Wool alcohol cream DAB/SR	22A200213	1
Caelo	Wool alcohol cream DAB/SR	230512	1
Caelo	Wool alcohol cream DAB/SR	23021303	1
Pharmachem / Phoenix	Wool alcohol cream DAB/SR	260413	2
Caelo	Wool alcohol cream DAB/SR	25091204	1
Euro OTC	Wool alcohol cream DAB/SR	2507217035	1
Pharmachem/Phönix	Wool alcohol cream DAB/SR	260413	1
Phoenix (Pharmachem Pöß. . .	Wool alcohol cream DAB/SR	260712	1
Gehe	Wool alcohol cream DAB/SR	272261	1
Bombastus	Wool alcohol cream DAB/SR	273633	1
Pharmachem.Pößneck	Wool alcohol cream DAB/SR	260712	1
Bombastus	Wool alcohol cream DAB/SR	274628	1
Gehe	Wool alcohol cream DAB/SR	274684	1
Alliance Healthcare	Wool alcohol cream DAB/SR	275909	1
Bombastus	Wool alcohol cream DAB/SR	274631	1
Bombastus	Wool alcohol cream DAB/SR	274629	1
Bombastus	Wool alcohol cream DAB/SR	274630	1
Caelo	Wool alcohol cream DAB/SR	274635	1
Gehe	Wool alcohol cream DAB/SR	274686	1
Gehe	Wool alcohol cream DAB/SR	274848	1
Bombastus	Wool alcohol cream DAB/SR	274849	1
Bombastus	Wool alcohol cream DAB/SR	275913	1
Euro OTC	Wool alcohol cream DAB/SR	275917	1
Bombastus	Wool alcohol cream DAB/SR	275918	1
Caelo	Wool alcohol cream DAB/SR	275988	1
Bombastus	Wool alcohol cream DAB/SR	275987	1
Bombastus	Wool alcohol cream DAB/SR	276216	1
Bombastus	Wool alcohol cream DAB/SR	276219	1
Bombastus	Wool alcohol cream DAB/SR	277093	1
Bombastus	Wool alcohol cream DAB/SR	277096	1
Bombastus	Wool alcohol cream DAB/SR	277097	2
Bombastus	Wool alcohol cream DAB/SR	277095	1
Bombastus	Wool alcohol cream DAB/SR	277770	1
Bombastus	Wool alcohol cream DAB/SR	277204	1
Bombastus	Wool alcohol cream DAB/SR	277769	1
Bombastus	Wool alcohol cream DAB/SR	27771	1
Bombastus	Wool alcohol cream DAB/SR	277854	1
Caelo	Wool alcohol cream DAB/SR	277855	1
Bombastus	Wool alcohol cream DAB/SR	278744	2
Bombastus	Wool alcohol cream DAB/SR	278749	1
Bombastus	Wool alcohol cream DAB/SR	278824	2
Bombastus	Wool alcohol cream DAB/SR	278828	2
Bombastus	Wool alcohol cream DAB/SR	278829	1
Bombastus	Wool alcohol cream DAB/SR	278832	1
Bombastus	Wool alcohol cream DAB/SR	278833	1
Bombastus	Wool alcohol cream DAB/SR	279014	1
Bombastus	Wool alcohol cream DAB/SR	279020	1
Gehe	Wool alcohol cream DAB/SR	279876	1
Bombastus	Wool alcohol cream DAB/SR	279874	1
Euro OTC	Wool alcohol cream DAB/SR	279873	1
Bombastus	Wool alcohol cream DAB/SR	279870	2
Bombastus	Wool alcohol cream DAB/SR	279876	1
Bombastus	Wool alcohol cream DAB/SR	279877	2
Bombastus	Wool alcohol cream DAB/SR	281504	1
Bombastus	Wool alcohol cream DAB/SR	281506	1
Gehe	Wool alcohol cream DAB/SR	280493	1
Bombastus	Wool alcohol cream DAB/SR	282239	1
Bombastus	Wool alcohol cream DAB/SR	282242	2
Gehe	Wool alcohol cream DAB/SR	282240	1

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Supplier	Substance	Batch	Spectra
Gehe	Wool alcohol cream DAB/SR	282242	1
Bombastus	Wool alcohol cream DAB/SR	282246	2
gehe	Wool alcohol cream DAB/SR	282748	1
Bombastus	Wool alcohol cream DAB/SR	282754	3
Bombastus	Wool alcohol cream DAB/SR	283575	1
Bombastus	Wool alcohol cream DAB/SR	284446	1
Bombastus	Wool alcohol cream DAB/SR	284445	1
Bombastus	Wool alcohol cream DAB/SR	284451	2
Gehe/Apomix/25.10.2013	Wool alcohol cream DAB/SR	28A210313	2
Caelo	Wool alcohol cream DAB/SR	29131-01371	1
Apomix	Wool alcohol cream DAB/SR	32A070312	1
Gehe	Wool alcohol cream DAB/SR	32A080413	1
Apomix	Wool alcohol cream DAB/SR	33A070312	1
Apomix	Wool alcohol cream DAB/SR	39A180413	3
All..Healthc./Apomix	Wool alcohol cream DAB/SR	41A020513	1
apomix/ANZAG/04.07.2013	Wool alcohol cream DAB/SR	4546233	1
Apomix/Phönix	Wool alcohol cream DAB/SR	47A040613	1
Apomix	Wool alcohol cream DAB/SR	47A040613	1
All..Healthc./Apomix	Wool alcohol cream DAB/SR	47A040613	1
Gehe	Wool alcohol cream DAB/SR	47a040613	1
Apomix	Wool alcohol cream DAB/SR	51A070512	1
Apomix	Wool alcohol cream DAB/SR	56A300713	1
Apomix	Wool alcohol cream DAB/SR	56A270613	1
Apomix	Wool alcohol cream DAB/SR	62A200612	1
Gehe	Wool alcohol cream DAB/SR	72A270813	1
Apomix	Wool alcohol cream DAB/SR	69A100712	1
Apomix	Wool alcohol cream DAB/SR	90A021012	1
Apomix/Noweda	Wool alcohol cream DAB/SR	81A260913	1
Gehe	Wool alcohol cream DAB/SR	80A010812	1
apomix PKH GmbH Halle	Wool alcohol cream DAB/SR	88A231013	1
Gehe	Wool alcohol cream DAB/SR	95A161012	1
Apomix	Wool alcohol cream DAB/SR	96A161012	1
Apomix	Wool alcohol cream DAB/SR	98A241012	1

- 56 453 spectra from 332 *Apo-Ident* customers from a total of 19 369 batches from a further 328 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 *Wool alcohol cream DAB/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 *Wool alcohol cream DAB/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	660	0	33 684
Type B	0	2798	22	60 774
Type C	0	1757	231	56 453

The substance/substance group *Wool alcohol cream DAB/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 % (> 99.9689 %)	100.0000 % (> 99.0909 %)
Type B	100.0000 % (> 99.9710 %)	99.2199 % (> 99.1135 %)
Type C	100.0000 % (> 99.5963 %)	88.3803 % (> 88.2294 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31229	32160	5.70	22.67
31248	31287	1.74	27.57
31271	31271	0.00	25.79
31287	31287	0.00	28.36
31447	31447	0.00	21.10
31455	31455	0.00	23.43
31481	31926	2.24	24.38
31923	31923	0.00	26.95
31926	31926	0.00	24.08
31928	31928	0.00	24.86
31930	31930	0.00	28.72
31933	31933	0.00	27.87
31934	31934	0.00	30.07
31937	31937	0.00	30.62
32160	32160	0.00	25.42
33140	33140	0.00	25.70

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Wool fat
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	30743-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Wool fat; Adeps lanae; Adeps lanae anhydricus

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Wool fat*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Wool fat	12122403	30743	40	20120514
Henry Lamotte	Wool fat	5320900	30925	40	20120608
Caelo	Wool fat	14086904	31479	40	20140321
Euro OTC	Wool fat	1403023-01	31533	40	AR-14-FG-012696-01
Caelo	Wool fat	15050902	31742	40	20150223
Euro OTC	Wool fat	1502024-01	31743	40	AR-16-FG-003762-01
Euro OTC	Wool fat	1601040	31847	40	20160127*
Caelo	Wool fat	15198802	31952	40	20150625

Validation samples

A total of 156 379 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 *Wool fat*. These samples are listed above in the [calibration samples](#) section.
- 34 024 spectra from a total of 790 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 220 spectra of 8 reference samples from the substance/substance group *Wool fat*.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Wool fat	1403023-01	31533 [†]	20
Caelo	Wool fat	15050902	31742 [†]	20
Euro OTC	Wool fat	1502024-01	31743 [†]	20
Euro OTC	Wool fat	1601040	31847 [†]	20
Caelo	Wool fat	15198802	31952 [†]	20
Caelo	Wool fat	152923	31998	40
Euro OTC	Wool fat	1607001	32459	40
Caelo	Wool fat	16221907	33111	40

- 63 374 spectra from a total of 1469 batches from further 439 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

*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.

[†]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*.

provided by the customer regarding manufacturer and batch number.

- 1108 spectra from 238 *Apo-Ident* customers from 224 batches from the substance/substance group *Wool fat*.

Supplier	Substance	Batch	Spectra
Caelo	Wool fat	13306203	10
Caelo	Wool fat	13306205	6
Caelo	Wool fat	14086903	14
Caelo	Wool fat	13398202	5
Caelo	Wool fat	14086906	14
Caelo	Wool fat	14086905	12
Caelo	Wool fat	14147902	15
Caelo	Wool fat	14147901	8
Caelo	Wool fat	14238006	10
Caelo	Wool fat	14238004	11
Caelo	Wool fat	14304501	15
Caelo	Wool fat	15198802	9
Caelo	Wool fat	15158401	14
Caelo	Wool fat	15198804	13
Caelo	Wool fat	16003901	10
Caelo	Wool fat	16003905	9
Anzag/Beiersdorf	Wool fat	15050902	1
Caelo	Wool fat	16163006	2
Caelo	Wool fat	16044302	12
Bomastus direkt	Wool fat	60081303	1
Bombastus	Wool fat	288711	1
henry lamotte	Wool fat	5528000	1
Bombastus	Wool fat	281849	1
henry lamotte	Wool fat	5690800	1
Henry Lamotte Oils	Wool fat	5787700	1
Bombastus	Wool fat	272421	1
Henry LAmotte Oils GmbH...	Wool fat	8002112002	1
Herbasinica	Wool fat	5264700	2
Caelo	Wool fat	1206702	1
GEHE	Wool fat	12036703	2
Caelo	Wool fat	12224405	15
Bombastus	Wool fat	260535	1
Caelo	Wool fat	12321803	11
Caelo	Wool fat	13039403	24
Caelo	Wool fat	1303403	1
henry lamotte oils	Wool fat	5264700	1
Caelo	Wool fat	12321807	2
Phoenix	Wool fat	13039403	1
Caelo	Wool fat	13039405	14
Caelo	Wool fat	13094905	15
Caelo	Wool fat	13213106	13
Caelo	Wool fat	13213107	13
Caelo	Wool fat	13213104	12
Caelo	Wool fat	13213105	8
Caelo	Wool fat	13306206	17
Caelo	Wool fat	13306207	15
Lamotte	Wool fat	5198200	1
henry lamotte	Wool fat	5375400	2
Lamotte/Anzag	Wool fat	5264700-3384310110	1
Henry Lamotte Oils	Wool fat	5448200	1
	Wool fat	5198200	1
henry lamotte	Wool fat	5520800	1
Bombastus	Wool fat	267377	2
Bombastus	Wool fat	268668	4

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Supplier	Substance	Batch	Spectra
Bombastus	Wool fat	254683	1
Bombastus	Wool fat	273197	3
Caelo	Wool fat	2061509	1
Caelo	Wool fat	4061402	1
Caelo	Wool fat	4101404	1
Caelo	Wool fat	316E-01056	1
Caelo	Wool fat	612211056	1
Caelo	Wool fat	8011509	1
Caelo	Wool fat	6111212	1
Caelo	Wool fat	7051401	1
Caelo	Wool fat	5081406	1
Caelo	Wool fat	11016905	1
Caelo	Wool fat	8061304	1
Caelo	Wool fat	11203902	2
Caelo	Wool fat	11261102	1
Caelo	Wool fat	11016906	1
Caelo	Wool fat	11031302	1
Caelo	Wool fat	11203903	1
Caelo	Wool fat	11261103	2
Noweda	Wool fat	11203903	2
Fagron	Wool fat	11L07-T01	1
Caelo	Wool fat	11261106	2
Caelo	Wool fat	11261105	2
Caelo	Wool fat	12006702	1
Caelo	Wool fat	12015603	8
Purren Apotheke	Wool fat	11261106	1
Caelo	Wool fat	12015604	4
Caelo	Wool fat	12015605	4
Caelo	Wool fat	12036702	5
Noweda/ 18.06.12 Caela	Wool fat	12015605	1
Noweda	Wool fat	12036702	1
Phönix 14.08.2012	Wool fat	12036703	1
Caelo	Wool fat	12036703	7
Caesar & Loretz GmbH	Wool fat	12036703	1
Caesar & Loretz GmbH, 4...	Wool fat	12036703	1
Caelo	Wool fat	1206703	1
Caelo	Wool fat	12036704	6
Caelo	Wool fat	12074502	5
Caelo	Wool fat	12074501	2
Caelo	Wool fat	12091301	1
Gehe	Wool fat	12122403	1
Caelo	Wool fat	12122403	13
Caesar & Loretz GmbH	Wool fat	12122403	1
Caelo	Wool fat	12122404	18
Anzag/13.02.2013	Wool fat	12122403	1
Caelo	Wool fat	12122406	12
Sanacorp	Wool fat	12122404	1
Caelo	Wool fat	12224403	6
Caelo	Wool fat	12224402	1
Caelo	Wool fat	1213E-01056	1
Caelo	Wool fat	12224404	17
Gehe	Wool fat	12224404	1
Noweda	Wool fat	12224404	4
Alliance Healthcare	Wool fat	12224404	1
vdl	Wool fat	12224404	1
Kehr	Wool fat	12224405	1
Caelo	Wool fat	12321801	2
Caelo	Wool fat	12321802	6
Caelo	Wool fat	1231802	1
Phönix 02.04.2013	Wool fat	12321805	1

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Supplier	Substance	Batch	Spectra
Caelo	Wool fat	12321805	9
Fagron	Wool fat	12H31-T01	1
Fagron	Wool fat	12K07-T51-00357	1
cesar&lorentz/Phönix	Wool fat	12321805	1
Caelo	Wool fat	13039402	10
Caesar & Loretz GmbH, 4. ...	Wool fat	13039402	1
Gehe	Wool fat	13039402	1
gehe 05.09.13	Wool fat	13039402	1
Alliance Healthcare	Wool fat	13039403	1
Gehe	Wool fat	13039403	1
Sanacorp	Wool fat	13039405	1
Caelo	Wool fat	13094903	12
Caelo	Wool fat	13094902	4
Caelo	Wool fat	13081206	1
Caelo	Wool fat	1309405	1
Caelo	Wool fat	1309211056	1
Caelo	Wool fat	13094904	1
Phönix	Wool fat	13213104	1
Caelo	Wool fat	1321305	1
Sanacorp	Wool fat	13213104	1
Caelo	Wool fat	1321307	1
Caelo	Wool fat	1321308	1
Caesar & Loretz GmbH	Wool fat	13213104	1
Gehe	Wool fat	13213104	1
Gehe 11.11.2013	Wool fat	13213104	1
Caesar&Loretz GmbH/Anzag	Wool fat	13213105	1
Noweda	Wool fat	13213107	1
Caelo	Wool fat	13213108	20
Caelo	Wool fat	132131104	1
Caelo	Wool fat	13303208	1
Caelo	Wool fat	13306204	6
gehe	Wool fat	13306204	1
Gehe 26.2.14	Wool fat	13306205	2
Phönix	Wool fat	13306205	1
Caesar & Loretz GmbH	Wool fat	13306205	1
Sanacorp	Wool fat	13306206	1
Caelo	Wool fat	13306208	16
Caelo	Wool fat	133062707	1
Caelo	Wool fat	13389202	1
Caelo	Wool fat	13398201	15
Caelo	Wool fat	1336205	1
Phönix	Wool fat	1336206	1
Phoenix	Wool fat	13398201	1
Sanacorp	Wool fat	13398202	1
noweda	Wool fat	13398202	1
Caelo	Wool fat	14086902	1
Phoenix	Wool fat	13398202	1
Caelo	Wool fat	13398291	1
Euro OTC	Wool fat	1403023-01	1
GEHE	Wool fat	14086903	1
Phönix	Wool fat	14086903	1
Caelo	Wool fat	14086904	8
Bergchemie	Wool fat	14086904	1
Sanacorp	Wool fat	14086904	1
Noweda	Wool fat	14086905	1
Berkel AHK	Wool fat	14086905	1
Caelo	Wool fat	14086907	6
Caelo	Wool fat	14111402	1
Caelo	Wool fat	14121204	1
Bombastus	Wool fat	14147902	1

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Supplier	Substance	Batch	Spectra
12/2015	Wool fat	14147902	1
Caelo	Wool fat	14147903	13
Caelo	Wool fat	14147905	1
Caelo	Wool fat	14238002	6
Caelo	Wool fat	14238001	2
Caesar&loretz,AHC	Wool fat	14238002	1
Caelo	Wool fat	14238003	5
Caesar & Loretz GmbH	Wool fat	14238002	1
AHD	Wool fat	14238002	2
AHDE 19,05,.2015	Wool fat	14238002	1
Sanacorp	Wool fat	14238004	1
Caelo	Wool fat	14238005	6
Caelo	Wool fat	14238008	12
Caelo	Wool fat	14238007	3
Euro OTC	Wool fat	14238007	1
Allianz Healthcare 22.0...	Wool fat	14238008	1
Caelo	Wool fat	14238009	10
Caelo	Wool fat	14238010	5
Caelo	Wool fat	142383	1
Caesar & Loretz GmbH	Wool fat	14304501	1
Caelo	Wool fat	14304504	3
Caelo	Wool fat	14304502	7
Fagron	Wool fat	14304502	1
Sanacorp	Wool fat	14304502	1
Caelo	Wool fat	1434502	1
Fagron	Wool fat	14B14-T03	1
Euro OTC	Wool fat	1502024-01	1
Caelo	Wool fat	15041306	1
Caelo	Wool fat	15031401	1
Caelo	Wool fat	1505090	1
Caelo	Wool fat	15050903	8
Caelo	Wool fat	15050902	3
Caesar & Loretz GmbH	Wool fat	15050902	1
Caleo	Wool fat	15050903	1
Caelo	Wool fat	15050904	7
Caesar & Loretz GmbH	Wool fat	15050903	1
Caelo	Wool fat	15050906	10
Caelo	Wool fat	15158402	22
Caelo	Wool fat	15158404	1
Caelo	Wool fat	15158405	8
Caelo	Wool fat	1518401	1
Caesar&Loretz/Noweda	Wool fat	15198802	1
Noweda/Caesar & Loretz ...	Wool fat	15198802	1
Caelo	Wool fat	15198803	9
Phoenix	Wool fat	15292316	1
Caelo	Wool fat	15292309	4
Caelo	Wool fat	15292311	1
Caelo	Wool fat	15292316	4
Caesar&Loretz GmbH	Wool fat	16003901	1
Noweda	Wool fat	16003901	1
Caelo	Wool fat	16003902	12
Phönix	Wool fat	16003905	1
Caelo	Wool fat	1603211056	1
Euro OTC	Wool fat	1601040-01	1
Caelo	Wool fat	16044303	5
Caelo	Wool fat	16044304	1
Gehe	Wool fat	16044306	1
Caelo	Wool fat	16044306	4
Caelo	Wool fat	16121308	1
Caelo	Wool fat	1613001	1

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Supplier	Substance	Batch	Spectra
Caelo	Wool fat	16163001	3
Caesar & Loretz GmbH Hi...	Wool fat	16163001	1
Caelo	Wool fat	16163002	3
GEHE	Wool fat	16163006	1
Caelo	Wool fat	16221902	1
Caelo	Wool fat	16221904	3
Caelo	Wool fat	18021502	1
Caelo	Wool fat	1914M1056	1
Caelo	Wool fat	16267201	1
Caelo	Wool fat	18041503	1
Caelo	Wool fat	2113U01056	1
Caelo	Wool fat	21071502	1
Caelo	Wool fat	24422111203903	1
Caelo	Wool fat	26061205	1
Bombastus	Wool fat	275888	1
Bombastus	Wool fat	283526	3
Bombastus	Wool fat	275889	2
Bombastus	Wool fat	281850	1
Bombastus	Wool fat	279840	2
Caelo	Wool fat	27091204	1
Bombastus	Wool fat	277470	1
Caelo	Wool fat	2814U-01056	1
Bombastus	Wool fat	288712	3
Bombastus	Wool fat	286362	2
Caelo	Wool fat	286362	1
Bombastus	Wool fat	290878	1
Bombastus	Wool fat	294438	1
Caelo	Wool fat	29041407	1
Bombastus	Wool fat	291339	1
Bombastus	Wool fat	295371	1
Bombastus	Wool fat	296321	2
Bombastus	Wool fat	297572	1
Caelo	Wool fat	30101311	1
Caelo	Wool fat	31011302	1
Caelo	Wool fat	3112U-01056	1
Caelo	Wool fat	3513U-01056	1
Caelo	Wool fat	4013Q1056	1
Caelo	Wool fat	412062-1-P	1
Caelo	Wool fat	3x13398202	1
Sanacorp	Wool fat	46/AKD1	1
Noweda	Wool fat	5065900	1
Caelo	Wool fat	46/AKD3	1
Sanacorp	Wool fat	46/AKD6	1
Caelo	Wool fat		2
Phönix	Wool fat	5100700	1
Anzag am 08.05.2012	Wool fat	5163200	1
Klenk	Wool fat	5132100	1
Caelo	Wool fat	5163200	1
Lamotte/ Sanacorp	Wool fat	5198200	2
Henry Lamotte Oils	Wool fat	5198200	2
Caelo	Wool fat	5211E-01056	1
Caelo	Wool fat	5212Q-01056	1
Henry Lamotte Oils	Wool fat	5253400	1
Lamotte/Sanacorp	Wool fat	5253400	1
Phoenix	Wool fat	5216400	1
Lamotte/Krieger	Wool fat	5264700	2
Noweda	Wool fat	5264700	3
Finze	Wool fat	5264700	2
Henry Lamotte Oils GmbH	Wool fat	5264700	1
Lamotte/Phönix	Wool fat	5264700	1

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Supplier	Substance	Batch	Spectra
phönix, 23.11.2012	Wool fat	5264700	1
Großhandel	Wool fat	5264700	1
Lamotte Sanacorp	Wool fat	5264700	1
Lamotte/Otto	Wool fat	5264700	1
Fagron	Wool fat	5264700	1
lamotte/anzag	Wool fat	5264700	1
Anzag 25.02.13 ek: 14,44EUR	Wool fat	5264700	1
Henry Lamotte Oils/Sana...	Wool fat	5320900	1
Gehe/ Lamotte	Wool fat	5375400	1
Gehe	Wool fat	5375400	2
Phönix	Wool fat	5375400	1
Lamotte	Wool fat	5320900	1
Noweda	Wool fat	5375400	1
Henry Lamotte Oils GmbH	Wool fat	5375400	1
Lamotte/Otto	Wool fat	5375400	3
Phoenix	Wool fat	5375400	2
Anzag	Wool fat	5375400	2
Caelo	Wool fat	5375400	1
Lamotte	Wool fat	5375400	2
Henry Lamotte/GEHE	Wool fat	5375400	1
Gehe 02.07.2013	Wool fat	5375400	2
NW/ Lamotte	Wool fat	5375400	1
Henry Lamotte Oils/ Now...	Wool fat	5375400	1
Henry Lamotte	Wool fat	5448200	3
Noweda	Wool fat	5448200	1
Sanacorp	Wool fat	5448200	3
Lamotte/Sanacorp	Wool fat	5448200	1
Henry Lamotte Oils GmbH	Wool fat	5448200	1
Lamotte/Phoenix	Wool fat	5448200	1
Lamotte Sanacorp	Wool fat	5448200	1
Caelo	Wool fat	5448200	1
Großhandel	Wool fat	5448200	1
Lamotte	Wool fat	5520800	1
Henry Lamotte	Wool fat	5520800	1
Henry Lamotte Oils/ Now...	Wool fat	5520800	2
Henry Lamotte Oils GmbH...	Wool fat	5520800	1
Lamotte/Sanacorp	Wool fat	5520800	1
Henry Lamotte Oils/ Gehe	Wool fat	5520800	2
Caelo	Wool fat	5520800	4
Phönix	Wool fat	5520800	1
Lamotte/Phoenix	Wool fat	5520800	2
Henry Lamotte Oils	Wool fat	5520800	1
Henry Lamotte Oils GmbH	Wool fat	5520800	1
Henry Lamotte/Noweda	Wool fat	5520800	1
Henry Lamotte Oils GmbH...	Wool fat	5520800	1
Alliance healthcare	Wool fat	5520800	1
Henry Lamotte	Wool fat	5520800	1
Henry Lamotte Oils GmbH...	Wool fat	5520800	1
Lamotte/gehe	Wool fat	5520800	1
Lamotte/Jenne 30.10.2014	Wool fat	5520800	1
GEHE 02.12.2014	Wool fat	5520800	1
Henry Lamotte / Anzag	Wool fat	5690800	3
Henry Lamotte Oils GmbH...	Wool fat	5690800	2
Henry Lamotte / Anzag	Wool fat	5650500	1
Henry Lamotte Oils GmbH...	Wool fat	5650500	1
Lamotte	Wool fat	5650500	1
Lamotte/Phönix	Wool fat	5650500	1
Henry Lamotte Oils GmbH	Wool fat	56908000	1
Henry Lamotte	Wool fat	5690800	2
Gehe	Wool fat	5763900	1

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Supplier	Substance	Batch	Spectra
Caelo	Wool fat	5727500	1
Henry Lamotte Oils / No...	Wool fat	5763900	1
Caelo	Wool fat	5763900	1
Lamotte/Ebert	Wool fat	5787700	1
Lamotte/Noweda	Wool fat	5787700	1
Henry Lamotte/Noweda	Wool fat	5787700	1
Lamotte/Otto	Wool fat	5787700	1
Lamotte/Phoenix	Wool fat	5787700	1
noweda/lamotte	Wool fat	5763900	1
Henry Lamotte Oils GmbH	Wool fat	5860600	1
Lamotte/Noweda	Wool fat	5860600	2
Henry Lamotte/Kehr	Wool fat	5909000	2
Caelo	Wool fat	5860600	1
Henry Lamotte	Wool fat	5860600	1
Henry Lamotte	Wool fat	5908900	1
henry lamotte oils Gmh/N	Wool fat	5908900	1
Lamotte/Noweda	Wool fat	5909000	2
Henry Lamotte	Wool fat	59090000	1
Henry Lamotte / Noweda	Wool fat	60011861002	1
Lamotte	Wool fat	6001861001	1
Henry Lamotte Oils/Phönix	Wool fat	6001861001	1
Henry Lamotte	Wool fat	6001861002	2
henry lamotte oils	Wool fat	6001861002	1
Lamotte/Anzag	Wool fat	6001861001	2
Henry Lamotte/Noweda	Wool fat	6001861002	1
Lamotte	Wool fat	6001861002	1
henry lamotte oils	Wool fat	6991861002	1
Caelo	Wool fat	82325376	1
Henry Lamotte/Noweda	Wool fat	8002112002	1

- 57 333 spectra from 332 *Apo-Ident* customers from a total of 19 870 batches from a further 328 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 *Wool fat* 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 *Wool fat* 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	34 024
Type B	0	220	0	63 374
Type C	0	1088	20	57 333

The substance/substance group *Wool fat* 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 % (> 99.9689 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9710 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.5963 %)	98.1949 % (> 97.9242 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30743	31743	5.08	18.60
30925	31847	5.26	18.50
31479	31743	1.94	15.37
31533	31533	0.00	17.19
31742	31743	3.19	17.99
31743	31743	0.00	17.01
31847	31847	0.00	19.22
31952	31743	1.99	17.78

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **Wormwood oil**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30846-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

Wormwood oil; Oleum absinthii

Special notes

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

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *Wormwood oil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Wormwood oil	11346603	30846	40	20111208
Caelo	Wormwood oil	13347703	31198	40	1403146
Caelo	Wormwood oil	13347704	31423	40	20131028
Caelo	Wormwood oil	13347704	31424	40	20131028

Validation samples

A total of 156 379 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 *Wormwood oil*. These samples are listed above in the [calibration samples](#) section.
- 34 184 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 40 spectra of 2 reference samples from the substance/substance group *Wormwood oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Wormwood oil	13347704	31423 [†]	20
Caelo	Wormwood oil	13347704	31424 [†]	20

- 63 554 spectra from a total of 1476 batches from further 439 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 2 batches from the substance/substance group *Wormwood oil*.

Supplier	Substance	Batch	Spectra
Caelo	Wormwood oil	12197809	1
Voegelé	Wormwood oil	2013109402	3

[†]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*.

- 58 437 spectra from 332 *Apo-Ident* customers from a total of 20 090 batches from a further 328 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 *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 *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	160	0	34 184
Type B	0	40	0	63 554
Type C	0	4	0	58 437

The substance/substance group *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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9711 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.5985 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30846	31198	4.83	82.77
31198	31198	0.00	81.89
31423	31198	2.05	83.20
31424	31198	1.61	83.18

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group	Ylang-ylang oil
Substance class	APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date	04/07/2017
Report number	31300-2017-07-04
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ylang-ylang oil; Oleum cananga odorata; Oleum ylang-ylang

Special notes

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

- Advice for the identification of essential oils : Some essential oils are listed in the class APIs & excipients, liquid/semi-solid (with analysis certificate) as well as in the class APIs & excipients, liquid/semi-solid (other).

Applicable documents

978-3-7692-5416-7	<i>European Pharmacopoeia 8th Edition, Basic Version 2014</i> [3]
Komm2.2.40	<i>Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident</i> [4]
AA004	<i>Erstellung und Validierung eines IdentModul-Updates</i>

Validation method

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

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

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

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
Caelo	Ylang-ylang oil	15101104	31791	40	9203
Caelo	Ylang-ylang oil	15101104	31860	40	20150330
Caelo	Ylang-ylang oil	15101109	32175	40	20150330
Caelo	Ylang-ylang oil	163148	33079	40	20161213*

Validation samples

A total of 156379 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 *Ylang-ylang oil*. These samples are listed above in the [calibration samples](#) section.
- 34184 spectra from a total of 795 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 180 spectra of 5 reference samples from the substance/substance group *Ylang-ylang oil*.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ylang-ylang oil	12040606	31300	40
Caelo	Ylang-ylang oil	14192905	31733	60
Caelo	Ylang-ylang oil	15101104	31791 [†]	20
Caelo	Ylang-ylang oil	15101104	31860 [†]	20
Caelo	Ylang-ylang oil	15101109	32350	40

- 63414 spectra from a total of 1473 batches from further 439 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.

*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.

[†]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*.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Ylang-ylang oil*.

Supplier	Substance	Batch	Spectra
Caelo	Ylang-ylang oil	23011502	1

- 58 440 spectra from 332 *Apo-Ident* customers from a total of 20 091 batches from a further 328 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	160	0	34 184
Type B	0	80	100	63 414
Type C	0	0	1	58 440

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 % (> 99.9690 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9710 %)	44.4444 % (> 42.7778 %)
Type C	100.0000 % (> 99.6053 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
31791	31791	0.00	56.51
31860	31791	2.71	58.30
32175	31791	5.76	60.10
33079	33079	0.00	49.05

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **1,3-butanediol**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30851-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

1,3-butanediol; 1,3-Butandiolium; Butylenglycolum

Special notes

When selecting the *1,3-butanediol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]

Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *1,3-butanediol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	1,3-butanediol	12J02-N07	30851	40	1402682
Fagron	1,3-butanediol	14G16-B01-296698	31594	40	20140804

Validation samples

A total of 156379 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 *1,3-butanediol*. These samples are listed above in the [calibration samples](#) section.
- 34264 spectra from a total of 796 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 20 spectra of 1 reference samples from the substance/substance group *1,3-butanediol*.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	1,3-butanediol	14G16-B01-296698	31594 [†]	20

- 63574 spectra from a total of 1476 batches from further 439 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 *1,3-butanediol*.

Supplier	Substance	Batch	Spectra
Caelo	1,3-butanediol	13L19-B03-291208	1
Fagron	1,3-butanediol	S6526964	1

[†]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*.

- 58 439 spectra from 332 *Apo-Ident* customers from a total of 20 090 batches from a further 328 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 *1,3-butanediol* 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 *1,3-butanediol* 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	34 264
Type B	0	20	0	63 574
Type C	0	2	0	58 439

The substance/substance group *1,3-butanediol* 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 % (> 99.9692 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9712 %)	100.0000 % (> 70.0000 %)
Type C	100.0000 % (> 99.6008 %)	n/a (n/a)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30851	30851	0.00	59.75
31594	30851	6.25	55.56

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

VALIDATION REPORT

IdentModul 1.3-2017-04

Validated substance/substance group **2-ethylhexyl laurate**
Substance class APIs & excipients, liquid/semi-solid (with analysis certificate)
Report date 04/07/2017
Report number 30849-2017-07-04
Executing company HiperScan GmbH
Weißeritzstraße 3
01067 Dresden
Germany

Relevant substance names

2-ethylhexyl laurate; 2-Ethylhexylislauromyristas; Cera liquida

Special notes

When selecting the *2-ethylhexyl laurate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-5416-7 *European Pharmacopoeia 8th Edition, Basic Version 2014* [3]
Komm2.2.40 *Erfüllung von 2.2.40 Ph. Eur. 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.

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 *2-ethylhexyl laurate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
apomix	2-ethylhexyl lau...	8013080312	30849	40	1405083
Caelo	2-ethylhexyl lau...	14129303	31373	40	20140429
Caelo	2-ethylhexyl lau...	14129304	31507	40	20140429
Caelo	2-ethylhexyl lau...	153825	31878	40	20151113*
Caelo	2-ethylhexyl lau...	163157	33086	40	20161124*

Validation samples

A total of 156 379 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 *2-ethylhexyl laurate*. These samples are listed above in the [calibration samples](#) section.
- 34 144 spectra from a total of 793 batches from further 224 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*.

These samples are allowed to originate from the same batch as calibration samples (*Type A*) as long as the package differs. In the following table spectra recorded from the same package as the corresponding calibration samples (*Type A*) are highlighted by [†].

- 92 spectra of 4 reference samples from the substance/substance group *2-ethylhexyl laurate*.

Supplier	Substance	Batch	Sample ID	Spectra
Pharmachem	2-ethylhexyl laurate	10610	30325	12
Caelo	2-ethylhexyl laurate	14129304	31507 [†]	20
Caelo	2-ethylhexyl laurate	153825	31878 [†]	20
Caelo	2-ethylhexyl laurate	163482	33087	40

- 63 502 spectra from a total of 1473 batches from further 439 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.

- 73 spectra from 39 *Apo-Ident* customers from 29 batches from the substance/substance group *2-ethylhexyl laurate*.

*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.

[†]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*.

Supplier	Substance	Batch	Spectra
Pharmachem	2-ethylhexyl laurate	50414	5
Pharmachem GmbH&Co.KG	2-ethylhexyl laurate	10515	1
Pharmachem/ Sanacorp	2-ethylhexyl laurate	10515	1
Pharmachem./Allianc.H.	2-ethylhexyl laurate	50414	1
Pharmachem/Sanacorp	2-ethylhexyl laurate	50414	1
Pharmachem/ Noweda	2-ethylhexyl laurate	50414	2
Caelo	2-ethylhexyl laurate	13252003	1
Caelo	2-ethylhexyl laurate	15382601	1
Caelo	2-ethylhexyl laurate	16143803	2
Caelo	2-ethylhexyl laurate	16143804	1
Apomix/Anzag	2-ethylhexyl laurate	3114U-03641	1
Phoenix/Apomix	2-ethylhexyl laurate	8015010115	1
Caelo	2-ethylhexyl laurate	16245001	1
Apomix/Sanacorp	2-ethylhexyl laurate	8015010115ZA48/15	1
apomix/Sanacorp	2-ethylhexyl laurate	8015050414	1
Caelo	2-ethylhexyl laurate	21091303	1
Caelo	2-ethylhexyl laurate	13018601	1
Caelo	2-ethylhexyl laurate		1
Gehe	2-ethylhexyl laurate	130312	2
apomix	2-ethylhexyl laurate	8325111111	1
Apomix/Noweda	2-ethylhexyl laurate	8014260413	1
Phönix Gotha	2-ethylhexyl laurate	131111	1
Caelo	2-ethylhexyl laurate	8014210112	1
Pharmachem/AHD	2-ethylhexyl laurate	10213	4
Caelo	2-ethylhexyl laurate	14129304	1
Caelo	2-ethylhexyl laurate	130312	1
Phönix Gotha	2-ethylhexyl laurate	10213	1
Apomix / Phönix	2-ethylhexyl laurate	40514	1
Pharmachem Pöckneck/Sana...	2-ethylhexyl laurate	10515	1
Pharmachem Pöckneck, GEHE	2-ethylhexyl laurate	10515	1
Pharmachem Pöckneck/Sana...	2-ethylhexyl laurate	50414	1
apomix/Noweda	2-ethylhexyl laurate	148-8013010616	1
apomix	2-ethylhexyl laurate	1488013010616	1
apomix	2-ethylhexyl laurate	148-8013010616	1
Euro OTC	2-ethylhexyl laurate	50414	2
Phoenix	2-ethylhexyl laurate	148-8013010616	1
PharmaChem	2-ethylhexyl laurate	50414	2
Apomix	2-ethylhexyl laurate	148-80130106ZA182/16	1
Apomix/Anzag	2-ethylhexyl laurate	813M-03324	1
apomix/ Phoenix	2-ethylhexyl laurate	8015050414	1
Apomix	2-ethylhexyl laurate	8015050414	1
Pharmachem/Phönix	2-ethylhexyl laurate	10213	1
apomix	2-ethylhexyl laurate	8015050414	1
Pharmachem / Phönix	2-ethylhexyl laurate	10213	1
Pharmachem GmbH	2-ethylhexyl laurate	10213	1
pharmachem GmbH Pöckneck	2-ethylhexyl laurate	10213	1
Apomix/Noweda	2-ethylhexyl laurate	8015050414ZA96/14	1
PKH Halle/Sanacorp	2-ethylhexyl laurate	8013120913	1
Pharmachem GmbH	2-ethylhexyl laurate	130312	1
Pharmachem/ Sanacorp	2-ethylhexyl laurate	130312	1
Pharmachem/ Noweda	2-ethylhexyl laurate	130312	1
Pharmachem GmbH&Co.KG	2-ethylhexyl laurate	130312	1
Pharmachem	2-ethylhexyl laurate	131111	4
Pharmachem/Noweda	2-ethylhexyl laurate	131111	2
Pharmachem GmbH	2-ethylhexyl laurate	131111	1
Pharmachem/Gehe	2-ethylhexyl laurate	131111	1
Bombastus	2-ethylhexyl laurate	221010	1

- 58 368 spectra from 332 *Apo-Ident* customers from a total of 20 064 batches from a further 328 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 *2-ethylhexyl laurate* 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 *2-ethylhexyl laurate* 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	34 144
Type B	0	89	3	63 502
Type C	0	67	6	58 368

The substance/substance group *2-ethylhexyl laurate* 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 % (> 99.9690 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9710 %)	96.7391 % (> 93.4783 %)
Type C	100.0000 % (> 99.5964 %)	91.7808 % (> 87.6712 %)

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
30849	30849	0.00	8.68
31373	31878	2.62	8.89
31507	31878	2.46	7.97
31878	31878	0.00	9.04
33086	33086	0.00	6.55

Such samples underline the statistical spread of the original reference substance, but cannot add any new characteristics of the substance.

Appendix A: Additional calibration samples (Type A)

Not required.

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 337 batches. From these 13 735 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
Anthroposan	Calendula mother...	0131106	40	not necessary
apomix	Benzalkonium chl...	05B150612	40	not necessary
apomix	Betamethasone va...	01B200912	40	not necessary
apomix	Clobatesol propi...	01B200912	40	not necessary
apomix	Dexamethasone 1%...	07A201011	30	not necessary
apomix	Dexamethasone 1%...	04A270513	40	not necessary
apomix	Epinephrine solu...	04A160712	40	not necessary
apomix	Hydrophilic metr...	09B201011	40	from supplier
apomix	Hydrophilic metr...	04B280411	40	from supplier
apomix	Hydrophilic metr...	08B290911	20	not necessary
apomix	Hydroxyethylcell...	12B240611	40	not necessary
apomix	Methylrosanilini...	03C200712	80	not necessary
apomix	Methylrosanilini...	01A260413	40	not necessary
apomix	Methylrosanilini...	05A200712	40	not necessary
apomix	Metronidazole 10...	06B120412	40	from supplier
apomix	Metronidazole 10...	17A271011	20	not necessary
apomix	Metronidazole 10...	07B110913	40	1403475
apomix	Oxytetracycline ...	02B160212	40	from supplier
apomix	Prednisolone 1% ...	01A100113	40	not necessary
apomix	Prednisolone 1% ...	05A191011	10	not necessary
apomix	Prednisolone 1% ...	07A031212	40	not necessary
apomix	Searing paste SR	08B060612	40	not necessary
apomix	Triamcinolone ac...	01B250811	10	not necessary
apomix	Triamcinolone ac...	09C111212	40	not necessary
apomix	Triamcinolone ac...	04A160212	40	from supplier
apomix	Triamcinolone ac...	01A210513	40	not necessary
apomix	Zinc oxide cream...	10B130712	20	from supplier
apomix	Zinc oxide oil S...	10B090712	40	from supplier
Audor	Vitamin F liposo...	AP307176FL	40	not necessary
Audor	Vitamin F liposo...	pending	40	not necessary
Bene	Tacholiniquin [®] 1...	350K121	40	from supplier
Bombastus	Bone oil	00238230	50	not necessary
Bombastus	Chinese cinnamon...	263892	40	AR-12-FG-006571-01
Bombastus	Propolis tinctur...	273005	40	not necessary
Bombastus	Propolis tinctur...	273005	40	not necessary
Bombastus	Zinc oxide cream...	00269349	20	not necessary
Bombastus	Zinc oxide cream...	00269409	40	not necessary
Bombastus	Zinc oxide lotio...	00243799	72	not necessary
Bombastus	Zinc oxide oil	00266696	40	not necessary
Bombastus	Zinc oxide oil DAC	00269769	40	from supplier
Bombastus	Zinc oxide oil S...	00269651	40	not necessary
Bombastus	Zinc oxide paste...	00256014	40	from supplier
Bombastus	Zinc oxide paste...	00267515	60	from supplier
Bombastus	Zinc paste DAB	00264410	40	from supplier
Caelo	Acorus tincture ...	11355109	40	not necessary
Caelo	Alcoholic liniment	13351909	40	not necessary
Caelo	Alcoholic liniment	10179425	40	not necessary
Caelo	Aloe vera oil (w...	110137-96542	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Angelica tinctur...	11015908	40	not necessary
Caelo	Arnica oil, fat	11086702	40	from supplier
Caelo	Arnica tincture ...	10362805	40	not necessary
Caelo	Arnica tincture ...	09358714	44	not necessary
Caelo	Aromatic tinctur...	09382716	10	not necessary
Caelo	Aromatic tinctur...	11355009	40	not necessary
Caelo	Basil oil	13395803	40	not necessary
Caelo	Basil oil	11035902	40	not necessary
Caelo	Basil oil	13153601	40	1404505
Caelo	Basil oil	11346902	40	not necessary
Caelo	Belladonna tinct...	10043003	74	not necessary
Caelo	Belladonna tinct...	11322601	40	not necessary
Caelo	Benzalkonium chl...	10190001	40	not necessary
Caelo	Benzalkonium chl...	12033409	40	not necessary
Caelo	Benzoic lard (st...	12063902	40	not necessary
Caelo	Birch tar	10327401	40	1402581
Caelo	Bitter orange pe...	09278014	40	not necessary
Caelo	Bitter orange pe...	82474059	40	AR-12-FG-008243-01
Caelo	Bitter orange pe...	11187201	40	not necessary
Caelo	Bitter tincture ...	11380108	60	not necessary
Caelo	Bitter tincture ...	11015709	40	not necessary
Caelo	Calendula oil, fat	14063403	40	not necessary
Caelo	Calendula oil, fat	13287203	40	1403102
Caelo	Calendula oil, fat	11183103	40	not necessary
Caelo	Calendula tinctu...	10052810	38	not necessary
Caelo	Campher oil 10%	13317402	40	1509155
Caelo	Campher oil 10%	13317402	60	not necessary
Caelo	Campher oil 10%	10203901	40	not necessary
Caelo	Camphor ointment	161773	40	20160711*
Caelo	Carmelite spirit	14001202	40	not necessary
Caelo	Carotene (ca. 4m...	12139305	40	1402564
Caelo	Cayenne pepper t...	11102412	40	not necessary
Caelo	Cayenne pepper t...	09165404	30	not necessary
Caelo	Chinchona bark t...	11275507	40	not necessary
Caelo	Cinchona bark ti...	10101502	40	not necessary
Caelo	Cinchona bark ti...	12056901	40	not necessary
Caelo	Coal tar solution	09345509	40	not necessary
Caelo	Coal tar solution	90392199	40	F 2009 000 986
Caelo	Coconut oil, har...	10122201	40	not necessary
Caelo	Comfrey root tin...	12054007	80	not necessary
Caelo	Comfrey tincture...	11121406	40	not necessary
Caelo	Food colorant bl...	12038601	40	not necessary
Caelo	Food colorant gr...	10320905	40	not necessary
Caelo	Food colorant gr...	12012503	40	not necessary
Caelo	Food colorant re...	11370506	40	not necessary
Caelo	Food colorant ye...	12022203	40	not necessary
Caelo	Food colorant ye...	12022212	40	not necessary
Caelo	Gentian tincture...	09092707	61	not necessary
Caelo	Gentian tincture...	pending	40	not necessary
Caelo	Gentian tincture...	80932238	40	AR-12-FG-007885-01
Caelo	Ginger oil	163186	40	20161213*
Caelo	Ginger tincture ...	11323801	40	not necessary
Caelo	Hawthorn tinctur...	11311816	40	not necessary
Caelo	Horse chestnut s...	11194605	40	1403541
Caelo	Horse chestnut s...	10346909	40	not necessary
Caelo	Hydrophobic tric...	4811E-03565	30	from supplier
Caelo	Hydroxyethylcell...	92968409	20	F 2009 000 984
Caelo	Hydroxyethylcell...	10292702	40	not necessary
Caelo	Hyoscyamus oil	162692	40	20160930*
Caelo	Iodine tincture	09356705	70	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Iron (III) chlor...	11232103	20	not necessary
Caelo	Larch terpine	161264	60	20160428*
Caelo	Lavender spirit	13300803	42	1403101
Caelo	Lavender spirit	11232303	40	not necessary
Caelo	Lavender spirit	13300803	60	not necessary
Caelo	Lily-of-the-vall...	10322804	40	not necessary
Caelo	Lime water	12055002	40	not necessary
Caelo	Marian thistle s...	11061106	40	from supplier
Caelo	Matricaria flowe...	10127005	50	not necessary
Caelo	Matricaria flowe...	10127009	20	not necessary
Caelo	Matricaria flowe...	11269917	40	not necessary
Caelo	Matricaria liqui...	09220405	41	not necessary
Caelo	Matricaria liqui...	12360310	40	not necessary
Caelo	Matricaria liqui...	12360306	40	not necessary
Caelo	Matricaria oil, ...	12189803	40	not necessary
Caelo	Matricaria oil, ...	810189803	20	not necessary
Caelo	Matricaria oil, ...	14001103	40	not necessary
Caelo	Melissa leaf tin...	11102807	40	not necessary
Caelo	Melissa leaf tin...	pending	40	not necessary
Caelo	Melissa leaf tin...	10105412	30	not necessary
Caelo	Myrrh tincture (...)	11260914	30	not necessary
Caelo	Nettle herb liqu...	14176902	40	1501199
Caelo	Nettle root tinc...	11187409	40	not necessary
Caelo	Nettle tincture ...	11108801	40	not necessary
Caelo	Opium tincture, ...	13394905	40	0914I-02461
Caelo	Opium tincture, ...	12020302	40	from supplier
Caelo	Orange flower oi...	13067707	40	1404598
Caelo	Orange flower oi...	13067705	40	not necessary
Caelo	Orange flower oi...	10267805	40	not necessary
Caelo	Orange flower wa...	12238104	40	not necessary
Caelo	Peanut oil, hydr...	13339803	40	not necessary
Caelo	Peanut oil, hydr...	11266907	60	AR-13-FG-010027-01
Caelo	Peppermint spiri...	11185902	70	from supplier
Caelo	Peppermint tinct...	11207405	40	not necessary
Caelo	Peppermint tinct...	10106502	39	not necessary
Caelo	Phosphoric acid ...	91297199	40	not necessary
Caelo	Plantain herb li...	11332613	40	not necessary
Caelo	Prednisolone ace...	13077701	100	not necessary
Caelo	Primrose root li...	13330110	60	not necessary
Caelo	Primrose root li...	12175307	100	1404596
Caelo	Propolis tinctur...	11269521	40	not necessary
Caelo	Propolis tinctur...	10305415	21	not necessary
Caelo	Pyroligneous aci...	12023203	40	not necessary
Caelo	Ratanhia tinctur...	09166415	40	not necessary
Caelo	Ratanhia tinctur...	pending	40	not necessary
Caelo	Rose water	11286002	20	not necessary
Caelo	Rosemary leaf ti...	09135005	40	not necessary
Caelo	Sage leaf liquid...	11372203	40	not necessary
Caelo	Sage leaf liquid...	10305313	40	not necessary
Caelo	Sage tincture (7...	09345013	72	not necessary
Caelo	Salicylic acid c...	153947	40	20151130*
Caelo	Salicylic acid c...	153946	40	20151130*
Caelo	Siam benzoin	395534-70585	40	not necessary
Caelo	Siam benzoin tin...	11239201	60	not necessary
Caelo	Siam benzoin tin...	13169905	42	1405623
Caelo	Spearmint water	11210003	40	not necessary
Caelo	St. John's wort ...	12076913	40	not necessary
Caelo	St. John's wort ...	13389218	40	not necessary
Caelo	St. John's wort ...	10197305	30	not necessary
Caelo	St. John's wort ...	11195217	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Caelo	Standardised cay...	13259103	20	not necessary
Caelo	Standardised cay...	12053902	40	not necessary
Caelo	Theriac	10122603	43	not necessary
Caelo	Thyme liquid ext...	10198601	41	not necessary
Caelo	Thyme liquid ext...	13273613	60	not necessary
Caelo	Thyme tincture (...)	10043113	40	not necessary
Caelo	Tormentil tinctu...	10067310	40	not necessary
Caelo	Tormentil tinctu...	11278301	40	not necessary
Caelo	Triamcinolone ac...	11258801	30	not necessary
Caelo	Triamcinolone ac...	11258801	40	not necessary
Caelo	Triamcinolone ac...	12250701	80	not necessary
Caelo	Valerian root li...	13343703	60	not necessary
Caelo	Valerian tinctur...	92588399	40	AR-12-FG-007325-02
Caelo	Valerian tinctur...	11254304	40	not necessary
Caelo	Valerian tinctur...	12113006	40	not necessary
Caelo	Valerian tinctur...	12113006	40	not necessary
Caelo	Valerian tinctur...	12196203	40	not necessary
Caelo	Vitamin A-palmit...	12132910	60	not necessary
Caelo	Vitamin A-palmit...	11178101	40	not necessary
Caelo	Vitamin A-palmit...	11178101	40	not necessary
Caelo	Witch hazel bark...	09371313	40	not necessary
Caelo	Witch hazel bark...	13357902	40	not necessary
Caelo	Witch hazel bark...	13357902	40	1407627
Caelo	Witch hazel leaf...	12165010	40	not necessary
Caelo	Witch hazel leaf...	12095402	40	1402497
Caelo	Witch hazel leaf...	10043706	40	not necessary
Caelo	Wormwood tinctur...	80681198	40	AR-12-FG-007926-01
Caelo	Wormwood tinctur...	12237901	40	not necessary
Caelo	Wormwood tinctur...	10010910	31	not necessary
Caelo	Yarrow herb tinc...	10169006	40	not necessary
Caelo	Zinc ointment DAB	10293402	30	not necessary
Caelo	Zinc ointment DAB	09347002	40	not necessary
Caelo	Zinc oxide lotio...	11263503	40	AR-12-FG-008390-01
Caelo	Zinc oxide lotio...	11263502	40	not necessary
Caelo	Zinc oxide lotio...	11013001	40	from supplier
Caelo	Zinc oxide lotio...	11281401	40	from supplier
Caelo	Zinc oxide lotio...	10340301	40	not necessary
Caelo	Zinc oxide lotio...	10340201	33	not necessary
Caelo	Zinc oxide lotio...	12065202	40	not necessary
Caelo	Zinc oxide lotio...	11281401	40	from supplier
Caelo	Zinc oxide oil DAC	12160002	40	not necessary
Caelo	Zinc oxide oil DAC	12289802	40	not necessary
Caelo	Zinc oxide paste...	00264201	40	not necessary
Caelo	Zinc oxide shaki...	11230101	40	not necessary
Caelo	Zinc paste DAB	00264409	40	not necessary
Caelo	Zinc paste DAB	11290801	40	not necessary
Caelo	Zinc paste DAB	12147801	40	not necessary
Caelo	Zinc paste DAB	11321701	30	not necessary
Caelo	Zinc paste, soft...	11006801	40	not necessary
Caelo	Zinc paste, soft...	12002802	40	not necessary
Caelo	Zinc paste, soft...	12378402	80	not necessary
Euro OTC	Capsaicin liquid...	1205038-01	40	not necessary
Euro OTC	Capsaicin liquid...	1205038-02	40	1406349
Fagron	Ammonium bitumin...	10F28-N06	20	not necessary
Fagron	Apricot aroma	11J11-N03	40	not necessary
Fagron	Apricot aroma	13D08-N08	30	1407103
Fagron	Carbomer gel 1%	1205D002	40	from supplier
Fagron	Hydrogen peroxid...	12A05-M07	40	not necessary
Fagron	Hydrogen peroxid...	174A270412	40	not necessary
Fagron	Mesulfen	11G12-N08	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Fagron	Methylrosanilini...	02A190511	40	not necessary
Fagron	Rose water	12A04-N04	40	not necessary
Fagron	Tretinoin soluti...	12C08-N14	40	not necessary
Fagron	Tretinoin soluti...	11K09-N03	40	not necessary
Fagron	Tretinoin soluti...	11K09-N03	40	not necessary
Fagron	Tretinoin soluti...	11K09-N03	40	not necessary
Fagron	Zinc paste DAB	12E22-T09	40	from supplier
Hedinger	Ammonia solution...	027132	10	from supplier
Hedinger	Ammonia solution...	027138	40	not necessary
Hedinger	Hydrogen peroxid...	301199	40	from supplier
Hedinger	Hydrogen peroxid...	0623498	40	from supplier
Hedinger	Sodium hypochlor...	025339	40	not necessary
Hedinger	Sodium hypochlor...	046359	31	from supplier
Henry Lamotte	Zinc oxide lotio...	5375600	40	not necessary
Henry Lamotte	Zinc paste, soft...	5374900	30	not necessary
Henry Lamotte	Zinc paste, soft...	5067100	40	from supplier
HerbaSinica	%Glycerol + prop...	002	80	not necessary
HerbaSinica	%Glycerol + prop...	001	80	not necessary
Ichthyol	Betamethason-V 1...	09D034	50	AR-12-FG-003630-01
Ichthyol	Clobetasol 0.5% ...	09D035	50	AR-12-FG-003627-01
Ichthyol	Clobetasol 0.5% ...	11D034	40	not necessary
Ichthyol	Gentamicin 1% Co...	09D002	50	AR-12-FG-003628-01
Ichthyol	Ichthyol® raw m...	11A075	20	not necessary
Ichthyol	Methoxsalen 0.00...	11D033	40	from supplier
Infectopharm	Hydrophobic tric...	S071003.1	70	from supplier
Infectopharm	Hydrophobic tric...	1410F-03565	30	from supplier
Infectopharm	Hydrophobic tric...	S091107.1	40	not necessary
Infectopharm	Hydrophobic tric...	S091106.1	40	from supplier
Infectopharm	Hydrophobic tric...	S091106.1	40	not necessary
Infectopharm	Hydrophobic tric...	S071007.1	40	not necessary
Kreuz-Apotheke	Aristarom Peach	60644	40	not necessary
Leyh Pharma	Methylrosanilini...	131711	40	not necessary
Madaus	Tormentil tincture	L0900294	30	not necessary
Maros	Aaron's rod moth...	U3029	40	not necessary
Maros	Abrotani mother ...	RU2276	40	not necessary
Maros	Angelica root ti...	06026712	40	not necessary
Maros	Angelica root ti...	06026712	40	not necessary
Maros	Anise fruit tinc...	6856	40	not necessary
Maros	Arnica flower li...	4965	40	not necessary
Maros	Arnica root moth...	U3606	40	not necessary
Maros	Artichoke leaf l...	1009	40	not necessary
Maros	Artichoke leaf t...	5367	40	not necessary
Maros	Ash bark mother ...	U3264	40	not necessary
Maros	Bearberry leaf t...	5377	40	not necessary
Maros	Bilberry leaf mo...	U3749	40	not necessary
Maros	Bitter candytuft...	5408	40	not necessary
Maros	Bittersweet stal...	U3320	40	not necessary
Maros	Black cohosh mot...	U3668	40	not necessary
Maros	Boldo leaf mothe...	U3502	30	not necessary
Maros	Bryony root moth...	U3269	40	not necessary
Maros	Burnet root moth...	U3600	40	not necessary
Maros	Cape aloe tinctu...	02026012	40	not necessary
Maros	Caraway seed tin...	08026612	40	not necessary
Maros	Cistus tincture ...	11025811	40	not necessary
Maros	Common broom mot...	R4688	40	not necessary
Maros	Common wormwood ...	U2448	40	not necessary
Maros	Coneflower herb...	U3041	40	not necessary
Maros	Devil's claw roo...	5573	30	not necessary
Maros	European golden ...	U3057	40	not necessary
Maros	Fennel fruit tin...	6996	40	not necessary

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Supplier	Substance	Batch	Spectra	Certificate
Maros	Figwort mother t...	U3623	40	not necessary
Maros	Ginkgo leaf moth...	U2834	40	not necessary
Maros	Golden rot herb ...	6737	40	not necessary
Maros	Hawthorn fruit m...	U3224	40	not necessary
Maros	Horehound herb m...	U2929	40	not necessary
Maros	Horse chestnut s...	U2882	40	not necessary
Maros	Juniper tincture...	1239	40	not necessary
Maros	Lovage root moth...	U3389	40	not necessary
Maros	Marian thistle f...	U3432	40	not necessary
Maros	Matricaria flowe...	U3347	40	not necessary
Maros	Matricaria liqui...	6615	20	not necessary
Maros	Melissa leaf liq...	6399	40	not necessary
Maros	Mistletoe mother...	U2932	40	not necessary
Maros	Monk's pepper fr...	U3476	40	not necessary
Maros	Motherwort herb ...	U2785	40	not necessary
Maros	Motherwort herb ...	6997	40	not necessary
Maros	Muira puama liqu...	3548	40	not necessary
Maros	Nettle mother ti...	U3633	40	not necessary
Maros	Pansy herb tinct...	40971	40	from supplier
Maros	Pansy mother tin...	pending	40	not necessary
Maros	Pelargonium root...	01028113	40	not necessary
Maros	Peppermint leaf ...	RU2432	40	not necessary
Maros	Primrose root ti...	03026212	40	not necessary
Maros	Primrose root ti...	03026212	40	not necessary
Maros	Ribwort plantain...	6736	40	not necessary
Maros	Robert herb moth...	U3720	40	not necessary
Maros	Rosemary leaf mo...	U3238	40	not necessary
Maros	St. John's wort ...	9712	40	not necessary
Maros	Standardised liq...	PH-226/12	20	not necessary
Maros	Strophanthus see...	01028513	40	not necessary
Maros	Sundew herb moth...	U3354	40	not necessary
Maros	Teasel root moth...	U3685	40	not necessary
Maros	Tetterwort mothe...	U3063	40	not necessary
Maros	Thyme liquid ext...	6869	40	not necessary
Maros	Valerian root li...	6398	40	not necessary
Maros	Walnut bark tinc...	1240	40	not necessary
Maros	Waterhorehound h...	U3388	40	not necessary
Maros	Willow bark tinc...	6865	40	not necessary
Maros	Wood violet moth...	U2222	40	not necessary
Maros	Yam mother tinct...	32210	40	not necessary
Otto Fischar	Hydrogen peroxid...	pending	40	not necessary
Phylak Sachse...	Malva silvestris...	2002012	30	not necessary
Phylak Sachse...	Rhus toxicodendr...	2908014	30	not necessary
Phylak Sachse...	Ruta graveolens...	2002012	30	not necessary
Ratiopharm	Corticoid-ratiop...	L30263	40	from supplier
Staufen-Pharm	Cocculus spag. z...	06.10.08	30	not necessary
Staufen-Pharm	Oxalic acid D30 ...	09.05.12	80	not necessary
pending	Dichloroacetic a...	pending	40	not necessary
pending	Zinc paste, soft...	pending	40	not necessary

*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 1899 batches. From these, 4618 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
AHD	Castor oil, hydrated	278661	1
AHD, 16.05.13	Zinc oxide oil DAC	13069701	23
alliance healthcare	Matricaria oil, fat	13204306	2
All..Healthc./Apomix	Hydrophilic metronida...	7B180713	6
Alliance Health	Zinc paste, soft DAB	278229	2
Alliance Healthcare	Hydrophobic triclosan...	S091202.1	6
Alliance Healthcare	Zinc paste, soft DAB	281118	1
Alliance Healthcare	Zinc paste, soft DAB	5374900	6
Alliance Healthcare/A...	Hydrophilic metronida...	11201113	1
Alliance Healthcare/A...	Hydrophilic metronida...	6B120613	4
AMH Niemann	Methylrosanilinium ch...	3A060612	1
AMH Niemann GmbH & Co...	Hydrophilic metronida...	4190413	1
AMH Niemann GmbH & Co...	Methylrosanilinium ch...	1b140213	1
AMH Niemann GmbH & Co...	Zinc oxide paste, sof...	25A310712	2
AMH Niemann GmbH& Co...	Hydroxyethylcellulose...	7B040313	1
AMH Niemann GmbH& Co...	Hydroxyethylcellulose...	13B310513	1
AMH Niemann GmbH,Halle	Hydroxyethylcellulose...	10B200412	2
AMH Niemann GmbH+Co Kg	Hydrophilic metronida...	5B170414	1
AMH Niemann/G	Oxytetracycline ointm...	4C300712	1
AMH Niemann/G	Oxytetracycline ointm...	2C160212	1
AMH Niemann/G	Oxytetracycline ointm...	1B200313	1
AMH Niemann/Noweda	Zinc oxide paste SR90	3A231012	1
AMH Niemann/Noweda	Zinc oxide paste SR90	1A150312	1
AMH/ Sanacorp	Zinc oxide paste, sof...	43B150811	1
AMH-Niemann GmbH & Co...	Hydroxyethylcellulose...	1B270112	1
AMH-Niemann GmbH & Co...	Hydroxyethylcellulose...	6C090312	1
AMH-Niemann GmbH & Co...	Hydroxyethylcellulose...	2C270112	1
amv niemann gmbh&co kg	Hydrophilic metronida...	4B060515	1
Anzag	Hydrophobic triclosan...	S021202.1	4
Anzag	Methylrosanilinium ch...	5A200712	1
Anzag	Methylrosanilinium ch...	1A140213	2
Anzag	Opium tincture, stand...	12006212	18
Anzag	Witch hazel bark water	11062810	1
Anzag	Zinc oxide paste, sof...	12207901	1
Anzag	Zinc oxide paste, sof...	12121501	1
Anzag	Zinc paste, soft DAB	12069101	6
Anzag am 06.02.2013	Sage tincture (70%) 1...	12196609	4
Anzag 19.12.2012	Castor oil, hydrated	273882	3
Anzag 26.11.12 ek:3,35	Orange flower water	12171703	1
Anzag 27.02.13	Hydroxyethylcellulose...	13009301	4
Anzag 27.12.12 ek:5,19	Campher oil 10%	12269502	10
Anzag 28.11.12	Zinc paste, soft DAB	12208001	9
Anzag 29.04.13 ek: 3,...	Castor oil, hydrated	13096304	1
Anzag ek:10.21EUR 27.08...	Alcoholic liniment	12103301	1
Anzag/Fischar	Hydrogen peroxide sol...	6313035	2
Anzag/Infectopharm	Hydrophobic triclosan...	S091206.1	7

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Supplier	Substance	Batch	Spectra
anzag/maros	Opium tincture, stand...	120061212	1
apomix	Benzalkonium chloride...	4a210515	1
apomix	Clobatesol propionate...	1A20213	1
apomix	Hydrogen peroxide sol...	6A070114	1
apomix	Hydrogen peroxide sol...	6A080116	1
apomix	Hydrogen peroxide sol...	231A160513	1
apomix	Hydrophilic metronida...	10C141013	1
apomix	Hydrophilic metronida...	11B221112	2
apomix	Hydrophilic metronida...	9B091013	2
apomix	Hydrophilic metronida...	5B020513	5
apomix	Hydroxyethylcellulose...	17B080713	1
apomix	Metronidazole 10% (no...	20B191211	1
apomix	Metronidazole 10% (no...	48170413	1
apomix	Metronidazole 10% (no...	5B150513	1
apomix	Searing paste SR	9B280613	2
apomix	Zinc oxide paste SR90	2A230811	1
apomix	Zinc oxide paste, sof...	34A231012	1
Apomix	Benzalkonium chloride...	3A170413	2
Apomix	Benzalkonium chloride...	6B060912	1
Apomix	Hydrogen peroxide sol...	227A160513	1
Apomix	Hydrophilic metronida...	8B110912	5
Apomix	Hydrophilic metronida...	1B030113	4
Apomix	Hydrophilic metronida...	1B190112	1
Apomix	Hydrophilic metronida...	2B220212	2
Apomix	Hydrophilic metronida...	2B220213	5
Apomix	Hydrophilic metronida...	4B270412	1
Apomix	Hydrophilic metronida...	9B041012	2
Apomix	Hydrophilic metronida...	10B251012	3
Apomix	Hydrophilic metronida...	11B201113	2
Apomix	Hydrophilic metronida...	3B140313	4
Apomix	Hydrophilic metronida...	8418213	2
Apomix	Hydroxyethylcellulose...	27B081113	1
Apomix	Hydroxyethylcellulose...	16B310513	2
Apomix	Hydroxyethylcellulose...	6B090312	1
Apomix	Hydroxyethylcellulose...	13B260413	3
Apomix	Hydroxyethylcellulose...	6D230514	1
Apomix	Hydroxyethylcellulose...	9B120413	1
Apomix	Hydroxyethylcellulose...	11B260413	1
Apomix	Hydroxyethylcellulose...	5B150213	3
Apomix	Hydroxyethylcellulose...	12B260413	1
Apomix	Hydroxyethylcellulose...	15B060712	1
Apomix	Hydroxyethylcellulose...	19B141011	1
Apomix	Hydroxyethylcellulose...	22B281011	1
Apomix	Hydroxyethylcellulose...	26B301112	1
Apomix	Hydroxyethylcellulose...	14B080612	1
Apomix	Metronidazole 10% (no...	1B020113	2
Apomix	Oxytetracycline ointm...	1A160212	1
Apomix	Zinc oxide cream 25% ...	13A040912	3
Apomix	Zinc oxide cream 25% ...	7B270513	1
Apomix	Zinc oxide oil DAC	26C190911	1
Apomix	Zinc oxide oil SR 90	5B250313	1
Apomix	Zinc oxide oil SR 90	6B150413	1
Apomix	Zinc oxide paste, sof...	3A090113	1
Apomix	Zinc oxide paste, sof...	12B140313	1
Apomix	Zinc paste, soft DAB	41B051212	1
Apomix	Zinc paste, soft DAB	13A040912	1
ApoMix	Hydrophilic metronida...	6B310512	3
Apomix / 11	Dexamethasone 1% (non...	4A270513	1
Apomix / 11	Triamcinolone acetoni...	10A051213	1
Apomix / 11	Triamcinolone acetoni...	9C111212	1

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Supplier	Substance	Batch	Spectra
Apomix / 11	Triamcinolone acetoni...	5A290713	2
Apomix / 11	Triamcinolone acetoni...	6A260813	2
APOMIX / 11	Prednisolone 1% (non-...	3A160813	1
Apomix / 20	Searing paste SR	12B150813	2
Apomix / 20	Triamcinolone acetoni...	8A190913	1
Apomix / 30	Triamcinolone acetoni...	7A170913	2
APOMIX / 30	Triamcinolone acetoni...	3A110613	1
Apomix / AHD	Hydroxyethylcellulose...	6B040313	1
Apomix / Phönix	Hydroxyethylcellulose...	21C090813	1
Apomix / Phönix	Hydroxyethylcellulose...	11B120413	1
Apomix Anzag	Hydrophilic metronida...	7B200712	5
Apomix direkt	Benzalkonium chloride...	4A110713	2
Apomix direkt	Benzalkonium chloride...	2B070313	1
APomix Phoenix	Searing paste SR	7B160513	1
apomix PKH	Hydrogen peroxide sol...	472A160913	1
apomix PKH	Hydroxyethylcellulose...	17B060712	1
apomix PKH	Hydroxyethylcellulose...	14B080612	1
apomix PKH	Hydroxyethylcellulose...	2B270112	1
apomix PKH	Hydroxyethylcellulose...	9C200412	1
apomix, Phönix	Zinc oxide paste, sof...	6A110213	2
Apomix/ 11	Triamcinolone acetoni...	4A040713	1
apomix/ Gehe	Methylrosanilinium ch...	2B290312	1
Apomix/ Noweda	Hydroxyethylcellulose...	5B090312	1
apomix/ Phoenix	Dexamethasone 1% (non...	2A220313	1
Apomix/ Phönix	Hydroxyethylcellulose...	19B090813	1
Apomix/ Sanacorp	Hydroxyethylcellulose...	19B080713	1
Apomix/ Sanacorp	Zinc oxide cream 25% ...	13B230813	1
Apomix/Anzag	Hydrogen peroxide sol...	67A300113	1
Apomix/Anzag	Hydroxyethylcellulose...	10C120413	1
Apomix/Anzag	Methylrosanilinium ch...	1B260413	1
Apomix/Gehe	Methylrosanilinium ch...	4B200712	1
Apomix/Noweda	Hydrophilic metronida...	8B290813	4
Apomix/Noweda	Hydroxyethylcellulose...	18B080713	1
Apomix/Noweda	Searing paste SR	11B010813	1
Apomix/Noweda	Searing paste SR	3B180213	2
Apomix/Noweda	Zinc oxide cream 25% ...	4A100413	1
apomix/phoenix	Betamethasone valerat...	13C031213	1
apomix/Phönix	Hydrophilic metronida...	11B20113	1
apomix/Phönix	Zinc oxide cream 25% ...	15B230913	1
Apomix/Phönix	Hydrophilic metronida...	12B111213	1
Apomix/Phönix	Zinc oxide paste, sof...	4A090113	3
Apotheke	Hydrogen peroxide sol...	9393	1
Apotheke	Hydrogen peroxide sol...	8350	1
Apotheke	Hydrogen peroxide sol...	7488	1
Apotheke	Hydrogen peroxide sol...	8352	1
Apotheke	Hydrogen peroxide sol...	8523	1
Apotheke	Hydrogen peroxide sol...	9467	1
Apotheke	Hydrogen peroxide sol...	9527	1
Apotheke	Hydrogen peroxide sol...	9949	1
Apotheke	Hydrogen peroxide sol...	8784	1
Apotheke	Hydrogen peroxide sol...	8195	1
Apotheke	Hydrogen peroxide sol...	8648	1
Apotheke	Opium tincture, stand...	10007013	15
Audor Pharma	Vitamin F liposomes (...)	AP302038FL	2
Audor Pharma	Vitamin F liposomes (...)	AP207152FL	2
Audor Pharma	Vitamin F liposomes (...)	AP307176FL	2
Audor Pharma	Zinc oxide lotion, aq...	13139402	9
Berkel AHK	Campher oil 10%	15028001	2
Bomba/AHD	Propolis tincture 20%	280337	1
Bombastus	Castor oil, hydrated	271754	2

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Supplier	Substance	Batch	Spectra
Bombastus	Castor oil, hydrated	273390	15
Bombastus	Castor oil, hydrated	26956512-13	1
Bombastus	Castor oil, hydrated	266593	1
Bombastus	Castor oil, hydrated	255179	1
Bombastus	Castor oil, hydrated	264468	1
Bombastus	Castor oil, hydrated	269565	3
Bombastus	Castor oil, hydrated	270580	5
Bombastus	Castor oil, hydrated	266591	1
Bombastus	Castor oil, hydrated	275938	1
Bombastus	Chinese cinnamon oil	269558	1
Bombastus	Chinese cinnamon oil	262660	1
Bombastus	Chinese cinnamon oil	263892	1
Bombastus	Hydroxyethylcellulose...	13190401	12
Bombastus	Propolis tincture 20%	275084	1
Bombastus	Propolis tincture 20%	276954	1
Bombastus	Propolis tincture 20%	281900	1
Bombastus	St. John's wort oil	282275	1
Bombastus	St. John's wort oil	272178	1
Bombastus	St. John's wort oil	279926	1
Bombastus	St. John's wort oil	293138	1
Bombastus	St. John's wort oil	275674	1
Bombastus	St. John's wort oil	283368	1
Bombastus	Zinc ointment DAB	275313	4
Bombastus	Zinc ointment DAB	282182	1
Bombastus	Zinc ointment DAB	30071602	1
Bombastus	Zinc ointment DAB	277335	2
Bombastus	Zinc oxide cream 25% ...	276966	2
Bombastus	Zinc oxide cream 25% ...	274259	1
Bombastus	Zinc oxide cream 25% ...	272491	1
Bombastus	Zinc oxide cream 25% ...	279248	1
Bombastus	Zinc oxide cream 25% ...	281755	1
Bombastus	Zinc oxide cream 25% ...	272490	1
Bombastus	Zinc oxide lotion, aq. ...	270608	1
Bombastus	Zinc oxide lotion, aq. ...	274933	1
Bombastus	Zinc oxide lotion, aq. ...	273199	2
Bombastus	Zinc oxide lotion, aq. ...	277579	1
Bombastus	Zinc oxide lotion, aq. ...	284632	1
Bombastus	Zinc oxide oil DAC	279564	1
Bombastus	Zinc oxide oil DAC	2608864	1
Bombastus	Zinc oxide oil DAC	301565	1
Bombastus	Zinc oxide oil DAC	264960	1
Bombastus	Zinc oxide oil DAC	286041	2
Bombastus	Zinc oxide oil DAC	278159	6
Bombastus	Zinc oxide oil DAC	274182	1
Bombastus	Zinc oxide oil DAC	282083	1
Bombastus	Zinc oxide oil DAC	269651	3
Bombastus	Zinc oxide oil DAC	267450	1
Bombastus	Zinc oxide oil DAC	269765	1
Bombastus	Zinc oxide oil DAC	269650	1
Bombastus	Zinc oxide oil DAC	269767	1
Bombastus	Zinc oxide oil DAC	273970	1
Bombastus	Zinc oxide oil DAC	273971	1
Bombastus	Zinc oxide oil SR 90	273973	6
Bombastus	Zinc oxide oil SR 90	269651	1
Bombastus	Zinc oxide oil SR 90	281661	1
Bombastus	Zinc oxide oil SR 90	277647	1
Bombastus	Zinc oxide paste SR90	273833	1
Bombastus	Zinc oxide paste SR90	282124	1
Bombastus	Zinc oxide paste SR90	266450	1
Bombastus	Zinc oxide paste SR90	276200	4

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Supplier	Substance	Batch	Spectra
Bombastus	Zinc oxide paste SR90	279384	1
Bombastus	Zinc oxide paste SR90	276198	1
Bombastus	Zinc oxide paste, sof...	273328	3
Bombastus	Zinc oxide paste, sof...	273329	4
Bombastus	Zinc oxide paste, sof...	273330	2
Bombastus	Zinc oxide paste, sof...	277662	1
Bombastus	Zinc oxide paste, sof...	271196	2
Bombastus	Zinc oxide paste, sof...	279586	2
Bombastus	Zinc oxide paste, sof...	267515	1
Bombastus	Zinc oxide paste, sof...	275031	1
Bombastus	Zinc oxide paste, sof...	281586	1
Bombastus	Zinc paste DAB	278272	2
Bombastus	Zinc paste DAB	278270	1
Bombastus	Zinc paste DAB	278273	2
Bombastus	Zinc paste DAB	276145	1
Bombastus	Zinc paste DAB	278861	1
Bombastus	Zinc paste DAB	27113603-15	1
Bombastus	Zinc paste DAB	280732	1
Bombastus	Zinc paste DAB	271136	1
Bombastus	Zinc paste DAB	280733	2
Bombastus	Zinc paste DAB	271135	2
Bombastus	Zinc paste DAB	271134	1
Bombastus	Zinc paste DAB	271133	1
Bombastus	Zinc paste DAB	287850	1
Bombastus	Zinc paste DAB	290176	1
Bombastus	Zinc paste DAB	291718	2
Bombastus	Zinc paste DAB	273890	1
Bombastus	Zinc paste DAB	62/13	1
Bombastus	Zinc paste DAB	276143	1
Bombastus	Zinc paste DAB	273894	1
Bombastus	Zinc paste DAB	278863	1
Bombastus	Zinc paste DAB	273893	2
Bombastus	Zinc paste DAB	278865	1
Bombastus	Zinc paste DAB	278864	3
Bombastus	Zinc paste DAB	278274	3
Bombastus	Zinc paste, soft DAB	278227	2
Bombastus	Zinc paste, soft DAB	275948	1
Bombastus	Zinc paste, soft DAB	278228	2
Bombastus	Zinc paste, soft DAB	271344	2
Bombastus	Zinc paste, soft DAB	271341	2
Bombastus	Zinc paste, soft DAB	274973	1
Bombastus	Zinc paste, soft DAB	276540	3
Bombastus	Zinc paste, soft DAB	281116	2
Bombastus	Zinc paste, soft DAB	280234	1
Bombastus	Zinc paste, soft DAB	280233	1
Bombastus	Zinc paste, soft DAB	278226	2
Bombastus	Zinc paste, soft DAB	278225	1
Bombastus	Zinc paste, soft DAB	278223	1
Bombastus	Zinc paste, soft DAB	276539	3
Bombastus	Zinc paste, soft DAB	276537	1
Bombastus	Zinc paste, soft DAB	276536	1
Bombastus	Zinc paste, soft DAB	270463	2
Bombastus	Zinc paste, soft DAB	265457	1
Bombastus	Zinc paste, soft DAB	282863	1
Bombastus	Zinc paste, soft DAB	274972	1
Bombastus	Zinc paste, soft DAB	274971	1
Bombastus	Zinc paste, soft DAB	293485	1
Bombastus	Zinc paste, soft DAB	11269801	1
Bombastus	Zinc paste, soft DAB	282859	1
Bombastus	Zinc paste, soft DAB	280235	1

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Supplier	Substance	Batch	Spectra
Bombastus	Zinc paste, soft DAB	271343	1
Bombastus	Zinc paste, soft DAB	267515	1
Bombastus	Zinc paste, soft DAB	282862	1
Bombastus	Zinc paste, soft DAB	267591	1
Bombastus	Zinc paste, soft DAB	266383	2
Bombastus	Zinc paste, soft DAB	264706	1
Bombastus	Zinc paste, soft DAB	266381	1
Bombastus	Zinc paste, soft DAB	267590	1
Bombastus	Zinc paste, soft DAB	270516	1
Bombastus	Zinc paste, soft DAB	271340	4
Bombastus	Zinc paste, soft DAB	281119	1
Bombastus	Zinc paste, soft DAB	281121	1
Bombastus	Zinc paste, soft DAB	270465	3
Bombastus	Zinc paste, soft DAB	271195	2
Bombastus	Zinc paste, soft DAB	271194	1
Bombastus	Zinc paste, soft DAB	281122	4
Bombastus	Zinc paste, soft DAB	270461	1
Bombastus	Zinc paste, soft DAB	273704	3
Brückenapotheke	Hydrophilic metronida...	414M-07001	1
Brückenapotheke	Hydrophilic metronida...	3313M-07001	1
Brückenapotheke	Hydrophilic metronida...	3113Q-07001	1
Brückenapotheke	Hydrophilic metronida...	3913E-07001	1
Brückenapotheke	Hydrophilic metronida...	5013A-07001	1
Brücken-Apotheke	Hydrophilic metronida...	4613M-07001	1
Caelo	Acorus tincture (70%)...	19121322	1
Caelo	Acorus tincture (70%)...	11355115	1
Caelo	Alcoholic liniment	12103319	2
Caelo	Alcoholic liniment	2612M-02925	1
Caelo	Alcoholic liniment	5213E2316	1
Caelo	Alcoholic liniment	445255	1
Caelo	Alcoholic liniment	34365645645	1
Caelo	Alcoholic liniment	2507212316	1
Caelo	Alcoholic liniment	12103312	1
Caelo	Alcoholic liniment	204312316	1
Caelo	Aloe vera oil (with a...	12033104	1
Caelo	Aloe vera oil (with a...	12033113	4
Caelo	Aloe vera oil (with a...	12033107	1
Caelo	Aloe vera oil (with a...	12033114	2
Caelo	Aloe vera oil (with a...	123033108	1
Caelo	Aloe vera oil (with a...	12383702	2
Caelo	Aloe vera oil (with a...	12383703	2
Caelo	Aloe vera oil (with a...	12383706	5
Caelo	Aloe vera oil (with a...	12033106	1
Caelo	Aloe vera oil (with a...	12033108	1
Caelo	Aloe vera oil (with a...	12033111	1
Caelo	Aloe vera oil (with a...	12033101	2
Caelo	Aloe vera oil (with a...	11014807	2
Caelo	Aloe vera oil (with a...	11014806	1
Caelo	Aloe vera oil (with a...	11014804	1
Caelo	Apricot aroma	14C19-B30-292291	1
Caelo	Arnica oil, fat	13186601	2
Caelo	Arnica oil, fat	Sanacorb	1
Caelo	Arnica oil, fat	13186602	2
Caelo	Arnica oil, fat	13042503	3
Caelo	Arnica oil, fat	12359703	1
Caelo	Arnica oil, fat	12088504	3
Caelo	Arnica oil, fat	13186604	1
Caelo	Arnica oil, fat	11096702	1
Caelo	Arnica tincture (70%)...	10362820	1
Caelo	Arnica tincture (70%)...	10341801	1

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Supplier	Substance	Batch	Spectra
Caelo	Arnica tincture (70%)...	26031301	1
Caelo	Arnica tincture (70%)...	20090312-4	1
Caelo	Arnica tincture (70%)...	12031001	1
Caelo	Arnica tincture (70%)...	12031008	1
Caelo	Arnica tincture (70%)...	12031017	8
Caelo	Arnica tincture (70%)...	1213A-02398	1
Caelo	Arnica tincture (70%)...	13094613	1
Caelo	Arnica tincture (70%)...	10362809	1
Caelo	Arnica tincture (70%)...	13094612	2
Caelo	Arnica tincture (70%)...	8111301	1
Caelo	Arnica tincture (70%)...	10362805	1
Caelo	Arnica tincture (70%)...	10362814	3
Caelo	Arnica tincture (70%)...	10362815	2
Caelo	Arnica tincture (70%)...	12031004	2
Caelo	Arnica tincture (70%)...	12031009	4
Caelo	Arnica tincture (70%)...	12031015	7
Caelo	Arnica tincture (70%)...	13094607	3
Caelo	Arnica tincture (70%)...	13094609	5
Caelo	Arnica tincture (70%)...	13094610	2
Caelo	Belladonna tincture, ...	12315104	1
Caelo	Belladonna tincture, ...	12315111	2
Caelo	Belladonna tincture, ...	11322601	1
Caelo	Belladonna tincture, ...	11322615	1
Caelo	Belladonna tincture, ...	13273004	1
Caelo	Belladonna tincture, ...	11322611	2
Caelo	Belladonna tincture, ...	12315101	1
Caelo	Benzalkonium chloride	13070201	1
Caelo	Benzalkonium chloride	13070206	6
Caelo	Benzalkonium chloride	12033403	2
Caelo	Benzalkonium chloride	12033411	1
Caelo	Benzalkonium chloride	13307902	1
Caelo	Benzoic lard (stabili...	12063902	1
Caelo	Bitter orange peel ti...	13003301	1
Caelo	Bitter orange peel ti...	13003302	1
Caelo	Bitter orange peel ti...	27072013	1
Caelo	Bitter orange peel ti...	12231906	2
Caelo	Bitter orange peel ti...	13003309	1
Caelo	Calendula mother tinc...	12117313	1
Caelo	Calendula mother tinc...	13142811	6
Caelo	Calendula oil, fat	122116904	1
Caelo	Calendula oil, fat	12373103	1
Caelo	Calendula oil, fat	13069603	1
Caelo	Calendula oil, fat	12216904	1
Caelo	Calendula oil, fat	13251002	3
Caelo	Calendula oil, fat	12216901	2
Caelo	Calendula oil, fat	12189903	3
Caelo	Calendula oil, fat	12308502	2
Caelo	Calendula oil, fat	13355701	1
Caelo	Calendula oil, fat	13251003	4
Caelo	Calendula oil, fat	13251002/1	1
Caelo	Calendula oil, fat	13185402	3
Caelo	Calendula oil, fat	13185401	2
Caelo	Calendula oil, fat	12373102	2
Caelo	Calendula oil, fat	nachprüfung	1
Caelo	Calendula oil, fat	12189901	1
Caelo	Calendula oil, fat	11183102	1
Caelo	Calendula oil, fat	12373101	2
Caelo	Calendula oil, fat	11274801	2
Caelo	Calendula oil, fat	12006802	4
Caelo	Calendula oil, fat	13069601	1

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Supplier	Substance	Batch	Spectra
Caelo	Calendula oil, fat	14001004	2
Caelo	Calendula tincture (7...	12117301	3
Caelo	Calendula tincture (7...	12117305	1
Caelo	Calendula tincture (7...	12117308	1
Caelo	Calendula tincture (7...	12117310	2
Caelo	Calendula tincture (7...	12117311	7
Caelo	Calendula tincture (7...	12117312	3
Caelo	Calendula tincture (7...	12117313	1
Caelo	Calendula tincture (7...	12117317	5
Caelo	Calendula tincture (7...	11332710	1
Caelo	Calendula tincture (7...	12117320	1
Caelo	Calendula tincture (7...	13142802	2
Caelo	Calendula tincture (7...	19061311	1
Caelo	Calendula tincture (7...	13142808	12
Caelo	Calendula tincture (7...	13142804	7
Caelo	Calendula tincture (7...	10260111	1
Caelo	Calendula tincture (7...	11143803	1
Caelo	Calendula tincture (7...	11332702	1
Caelo	Campher oil 10%	13317402	10
Caelo	Campher oil 10%	15338205	1
Caelo	Campher oil 10%	15338202	2
Caelo	Campher oil 10%	15028002	1
Caelo	Campher oil 10%	14139202	3
Caelo	Campher oil 10%	12269501	1
Caelo	Campher oil 10%	15208001	1
Caelo	Campher oil 10%	15338201	1
Caelo	Campher oil 10%	18082015A	1
Caelo	Campher oil 10%	13043901	2
Caelo	Campher oil 10%	13317401	2
Caelo	Campher oil 10%	15028003	1
Caelo	Campher oil 10%	15028004	2
Caelo	Campher oil 10%	15028003	1
Caelo	Campher oil 10%	14139202	2
Caelo	Carbomer gel 1%	1102D002	1
Caelo	Carotene (ca. 4m IU)	13008404	1
Caelo	Castor oil, hydrated	12114606	1
Caelo	Castor oil, hydrated	11260603	2
Caelo	Castor oil, hydrated	11260609	3
Caelo	Castor oil, hydrated	4101201	1
Caelo	Castor oil, hydrated	8061201	1
Caelo	Castor oil, hydrated	11359502	2
Caelo	Castor oil, hydrated	11359507	1
Caelo	Castor oil, hydrated	11359508	6
Caelo	Castor oil, hydrated	12042103	1
Caelo	Castor oil, hydrated	12071101	1
Caelo	Castor oil, hydrated	12114605	2
Caelo	Castor oil, hydrated	1304013-01	1
Caelo	Castor oil, hydrated	11260604	1
Caelo	Castor oil, hydrated	141200-02	1
Caelo	Castor oil, hydrated	12114602	3
Caelo	Castor oil, hydrated	25011301	1
Caelo	Castor oil, hydrated	16071201	1
Caelo	Castor oil, hydrated	14199604	1
Caelo	Castor oil, hydrated	11359501	2
Caelo	Castor oil, hydrated	291722	1
Caelo	Castor oil, hydrated	1112002-01	1
Caelo	Cayenne pepper tinctu...	12207111	2
Caelo	Cayenne pepper tinctu...	11102425	1
Caelo	Cayenne pepper tinctu...	11102419	1
Caelo	Cayenne pepper tinctu...	13072013	1

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Supplier	Substance	Batch	Spectra
Caelo	Cinchona bark tinctur...	13069808	1
Caelo	Coal tar solution	90391069	2
Caelo	Coal tar solution	24131-01799	1
Caelo	Coal tar solution	nachprüfung	1
Caelo	Coal tar solution	12286103	16
Caelo	Coal tar solution	9345406	1
Caelo	Coal tar solution	9345509	2
Caelo	Coal tar solution	9345510	1
Caelo	Coal tar solution	27071207	1
Caelo	Coal tar solution	15203703	1
Caelo	Coal tar solution	9039201	1
Caelo	Coal tar solution	9345507	1
Caelo	Coal tar solution	113192017	1
Caelo	Coal tar solution	11319203	1
Caelo	Coal tar solution	11319207	12
Caelo	Coal tar solution	11319209	1
Caelo	Coal tar solution	13193703	2
Caelo	Coal tar solution	13193713	1
Caelo	Coal tar solution	14331401	1
Caelo	Coal tar solution	14331509	1
Caelo	Coconut oil, hardened	13010804	1
Caelo	Coconut oil, hardened	11379517	1
Caelo	Coconut oil, hardened	11379511	1
Caelo	Coconut oil, hardened	11379510	2
Caelo	Coconut oil, hardened	613E-07004	1
Caelo	Coconut oil, hardened	13010808	2
Caelo	Comfrey root tincture...	11121314	2
Caelo	Comfrey root tincture...	12054008	1
Caelo	Comfrey root tincture...	12054012	2
Caelo	Comfrey tincture, cle...	4512E-02482	1
Caelo	Comfrey tincture, cle...	11121406	1
Caelo	Comfrey tincture, cle...	12177001	3
Caelo	Comfrey tincture, cle...	12177005	1
Caelo	Comfrey tincture, cle...	14298513	1
Caelo	Food colorant blue (E...	12322306	1
Caelo	Food colorant blue (E...	12038601	1
Caelo	Gentian tincture (70%...	11220506	1
Caelo	Gentian tincture (70%...	12035507	4
Caelo	Gentian tincture (70%...	13036405	4
Caelo	Gentian tincture (70%...	10334609	2
Caelo	Gentian tincture (70%...	11220504	1
Caelo	Gentian tincture (70%...	13036409	2
Caelo	Gentian tincture (70%...	4109M-02442	1
Caelo	Ginger tincture (70%)...	11323810	1
Caelo	Ginger tincture (70%)...	11053812	1
Caelo	Hawthorn tincture of ...	12211008	1
Caelo	Horse chestnut seed l...	12293604	1
Caelo	Horse chestnut seed l...	11194611	2
Caelo	Horse chestnut seed t...	12295308	1
Caelo	Hydrogen peroxide sol...	7575	1
Caelo	Hydrogen peroxide sol...		1
Caelo	Hydrogen peroxide sol...	610093	1
Caelo	Hydrogen peroxide sol...	12091302	1
Caelo	Hydrogen peroxide sol...	1003	1
Caelo	Hydrophobic triclosan...	S0211201.1	1
Caelo	Hydrophobic triclosan...	3131-07001	1
Caelo	Hydrophobic triclosan...	2111310005	1
Caelo	Hydroxyethylcellulose...	22061204	1
Caelo	Hydroxyethylcellulose...	11341501	1
Caelo	Hydroxyethylcellulose...	12351502	4

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Supplier	Substance	Batch	Spectra
Caelo	Hydroxyethylcellulose...	12351501	5
Caelo	Hydroxyethylcellulose...	12320601	5
Caelo	Hydroxyethylcellulose...	12244002	5
Caelo	Hydroxyethylcellulose...	12219501	4
Caelo	Hydroxyethylcellulose...	12219302	4
Caelo	Hydroxyethylcellulose...	12219201	6
Caelo	Hydroxyethylcellulose...	12209201	1
Caelo	Hydroxyethylcellulose...	2101201	1
Caelo	Hydroxyethylcellulose...	13009303	3
Caelo	Hydroxyethylcellulose...	13286301	3
Caelo	Hydroxyethylcellulose...	13286201	3
Caelo	Hydroxyethylcellulose...	13286101	5
Caelo	Hydroxyethylcellulose...	1319401	1
Caelo	Hydroxyethylcellulose...	13190901	3
Caelo	Hydroxyethylcellulose...	13190801	5
Caelo	Hydroxyethylcellulose...	13009501	10
Caelo	Hydroxyethylcellulose...	13021302	1
Caelo	Hydroxyethylcellulose...	13084402	10
Caelo	Hydroxyethylcellulose...	13084403	10
Caelo	Hydroxyethylcellulose...	13084404	13
Caelo	Hydroxyethylcellulose...	13190701	4
Caelo	Hydroxyethylcellulose...	2101203	1
Caelo	Hydroxyethylcellulose...	11011402	1
Caelo	Hydroxyethylcellulose...	11264501	1
Caelo	Hydroxyethylcellulose...	11341701	1
Caelo	Hydroxyethylcellulose...	11341801	4
Caelo	Hydroxyethylcellulose...	11363302	1
Caelo	Hydroxyethylcellulose...	11363401	1
Caelo	Hydroxyethylcellulose...	12071501	3
Caelo	Hydroxyethylcellulose...	12071701	2
Caelo	Hydroxyethylcellulose...	12128001	4
Caelo	Hydroxyethylcellulose...	12128201	5
Caelo	Hydroxyethylcellulose...	12128202	2
Caelo	Hydroxyethylcellulose...	12071401	2
Caelo	Hydroxyethylcellulose...	10111203	1
Caelo	Hydroxyethylcellulose...	3286101	1
Caelo	Hydroxyethylcellulose...	3786917	1
Caelo	Hydroxyethylcellulose...	4091303	1
Caelo	Hydroxyethylcellulose...	5121205	1
Caelo	Hydroxyethylcellulose...	6051303	1
Caelo	Hydroxyethylcellulose...	6061307	1
Caelo	Hydroxyethylcellulose...	1219401	1
Caelo	Hydroxyethylcellulose...	10111202	1
Caelo	Hydroxyethylcellulose...	8101303	1
Caelo	Hydroxyethylcellulose...	6121303	1
Caelo	Hydroxyethylcellulose...	6121301	1
Caelo	Hydroxyethylcellulose...	6061308	1
Caelo	Hydroxyethylcellulose...	13286401	1
Caelo	Hydroxyethylcellulose...	29061302	1
Caelo	Hydroxyethylcellulose...	30071301	1
Caelo	Hydroxyethylcellulose...	30071302	1
Caelo	Hydroxyethylcellulose...	17101201	1
Caelo	Hydroxyethylcellulose...	16061204	1
Caelo	Hydroxyethylcellulose...	15101311	1
Caelo	Hydroxyethylcellulose...	14066401	2
Caelo	Hydroxyethylcellulose...	14081202	1
Caelo	Hydroxyethylcellulose...	14081203	1
Caelo	Hydroxyethylcellulose...	14111307	1
Caelo	Hydroxyethylcellulose...	14111308	1
Caelo	Hydroxyethylcellulose...	14200101	1

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Supplier	Substance	Batch	Spectra
Caelo	Hydroxyethylcellulose...	29061301	1
Caelo	Hydroxyethylcellulose...	24011404	1
Caelo	Hydroxyethylcellulose...	24011403	1
Caelo	Hydroxyethylcellulose...	24011402	1
Caelo	Hydroxyethylcellulose...	23041305	1
Caelo	Hydroxyethylcellulose...	21111304	1
Caelo	Hydroxyethylcellulose...	21121201	1
Caelo	Hydroxyethylcellulose...	20071204	1
Caelo	Hydroxyethylcellulose...	29011301	1
Caelo	Hydroxyethylcellulose...	17101206	1
Caelo	Hydroxyethylcellulose...	17101207	1
Caelo	Hydroxyethylcellulose...	26101205	1
Caelo	Hydroxyethylcellulose...	26031306	1
Caelo	Hydroxyethylcellulose...	25091209	1
Caelo	Hydroxyethylcellulose...	14066301	1
Caelo	Hydroxyethylcellulose...	13393301	1
Caelo	Hydroxyethylcellulose...	13286801	2
Caelo	Hydroxyethylcellulose...	13286601	5
Caelo	Iodine tincture	11303104	1
Caelo	Iodine tincture	12285903	1
Caelo	Iodine tincture	12285906	3
Caelo	Iodine tincture	13193501	1
Caelo	Iodine tincture	12285902	1
Caelo	Iodine tincture	28061302	1
Caelo	Iodine tincture	24011405	1
Caelo	Iodine tincture	14111310	1
Caelo	Iodine tincture	14111309	1
Caelo	Iodine tincture	13193503	1
Caelo	Iodine tincture	13193502	1
Caelo	Iodine tincture	5021402	1
Caelo	Iodine tincture	5021308	1
Caelo	Iodine tincture	2101302	1
Caelo	Iodine tincture	9356601	1
Caelo	Iodine tincture	1071303	1
Caelo	Iodine tincture	12285901	1
Caelo	Lard	11263706	1
Caelo	Lard	11263714	1
Caelo	Lard	11379606	1
Caelo	Lard	11379605	2
Caelo	Lard	11263707	1
Caelo	Lard	11263715	1
Caelo	Lavender spirit	13166502	1
Caelo	Lavender spirit	13300803	2
Caelo	Lime water	13028602	1
Caelo	Marian thistle seed t...	12043822	1
Caelo	Marian thistle seed t...	13044304	1
Caelo	Marian thistle seed t...	11061110	1
Caelo	Matricaria flower tin...	11269911	2
Caelo	Matricaria flower tin...	11269924	1
Caelo	Matricaria flower tin...	11269905	1
Caelo	Matricaria flower tin...	11269917	3
Caelo	Matricaria flower tin...	12111305	1
Caelo	Matricaria flower tin...	24091208	1
Caelo	Matricaria flower tin...	1794290	1
Caelo	Matricaria flower tin...	14078402	1
Caelo	Matricaria flower tin...	13142803	1
Caelo	Matricaria flower tin...	13044206	1
Caelo	Matricaria flower tin...	13044202	1
Caelo	Matricaria flower tin...	11011307	1
Caelo	Matricaria flower tin...	3051310	1

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Supplier	Substance	Batch	Spectra
Caelo	Matricaria flower tin...	3081201	1
Caelo	Matricaria flower tin...	9061201	1
Caelo	Matricaria flower tin...	11011303	1
Caelo	Matricaria flower tin...	11011304	1
Caelo	Matricaria liquid ext...	10305319	1
Caelo	Matricaria liquid ext...	10382713	1
Caelo	Matricaria liquid ext...	10382716	3
Caelo	Matricaria liquid ext...	11303606	2
Caelo	Matricaria liquid ext...	12254803	1
Caelo	Matricaria liquid ext...	12360303	2
Caelo	Matricaria liquid ext...	1382716	1
Caelo	Matricaria liquid ext...	12254801	1
Caelo	Matricaria liquid ext...	12360310	3
Caelo	Matricaria liquid ext...	12360306	1
Caelo	Matricaria oil, fat	11261506	1
Caelo	Matricaria oil, fat	1218903	1
Caelo	Matricaria oil, fat	12372903	5
Caelo	Melissa leaf tincture...	11011305	1
Caelo	Melissa leaf tincture...	10105412	1
Caelo	Melissa leaf tincture...	27111307	1
Caelo	Melissa leaf tincture...	5121303	1
Caelo	Melissa leaf tincture...	12206214	3
Caelo	Melissa leaf tincture...	12206218	3
Caelo	Melissa leaf tincture...	11102812	1
Caelo	Melissa leaf tincture...	3051307	1
Caelo	Myrrh tincture (90%) ...	12197204	2
Caelo	Myrrh tincture (90%) ...	12197303	11
Caelo	Myrrh tincture (90%) ...	12197305	7
Caelo	Myrrh tincture (90%) ...	13273302	8
Caelo	Myrrh tincture (90%) ...	13273303	4
Caelo	Myrrh tincture (90%) ...	133273301	1
Caelo	Myrrh tincture (90%) ...	2002312460	2
Caelo	Myrrh tincture (90%) ...	12197107	2
Caelo	Myrrh tincture (90%) ...	11260916	2
Caelo	Myrrh tincture (90%) ...	12197105	12
Caelo	Myrrh tincture (90%) ...	11260914	5
Caelo	Myrrh tincture (90%) ...	11260909	3
Caelo	Myrrh tincture (90%) ...	13273301	7
Caelo	Myrrh tincture (90%) ...	12197103	2
Caelo	Myrrh tincture (90%) ...	12197104	1
Caelo	Myrrh tincture (90%) ...	20101012-1	1
Caelo	Myrrh tincture (90%) ...	24081209	1
Caelo	Myrrh tincture (90%) ...	2704212460	1
Caelo	Myrrh tincture (90%) ...	3101212460	1
Caelo	Myrrh tincture (90%) ...	614M2460	1
Caelo	Myrrh tincture (90%) ...	11019809	1
Caelo	Myrrh tincture (90%) ...	nachprüfung	1
Caelo	Myrrh tincture (90%) ...	13273404	1
Caelo	Myrrh tincture (90%) ...	12197112	3
Caelo	Myrrh tincture (90%) ...	20111214	1
Caelo	Myrrh tincture (90%) ...	230312	1
Caelo	Myrrh tincture (90%) ...	2913M2460	2
Caelo	Myrrh tincture (90%) ...	45132U2460	2
Caelo	Myrrh tincture (90%) ...	10112306	1
Caelo	Myrrh tincture (90%) ...	11019810	1
Caelo	Myrrh tincture (90%) ...	11260908	1
Caelo	Myrrh tincture (90%) ...	11260910	1
Caelo	Myrrh tincture (90%) ...	11260918	3
Caelo	Myrrh tincture (90%) ...	1910211095	1
Caelo	Myrrh tincture (90%) ...	12197106	1

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Supplier	Substance	Batch	Spectra
Caelo	Nettle root tincture ...	12341302	1
Caelo	Nettle root tincture ...	11187409	1
Caelo	Nettle tincture (70%)...	11108810	1
Caelo	Nettle tincture (70%)...	1108810	1
Caelo	Opium tincture, stand...	5008715	1
Caelo	Opium tincture, stand...	5005712	8
Caelo	Opium tincture, stand...	4007614	4
Caelo	Opium tincture, stand...	3071303	1
Caelo	Opium tincture, stand...	2007414	1
Caelo	Opium tincture, stand...	2007314	1
Caelo	Opium tincture, stand...	8061301	1
Caelo	Opium tincture, stand...	13144011	1
Caelo	Opium tincture, stand...	13144010	1
Caelo	Opium tincture, stand...	13144005	1
Caelo	Opium tincture, stand...	13144004	1
Caelo	Opium tincture, stand...	12380307	1
Caelo	Opium tincture, stand...	12380302	1
Caelo	Opium tincture, stand...	12162608	1
Caelo	Opium tincture, stand...	12162602	1
Caelo	Opium tincture, stand...	12121305	1
Caelo	Opium tincture, stand...	13260602	1
Caelo	Opium tincture, stand...	30031301	1
Caelo	Opium tincture, stand...	25071303	1
Caelo	Opium tincture, stand...	25071302	1
Caelo	Opium tincture, stand...	24011406	1
Caelo	Opium tincture, stand...	22031302	1
Caelo	Opium tincture, stand...	16121304	1
Caelo	Opium tincture, stand...	14108510	1
Caelo	Opium tincture, stand...	14108504	1
Caelo	Opium tincture, stand...	13394902	1
Caelo	Opium tincture, stand...	10011404	1
Caelo	Opium tincture, stand...	8061302	1
Caelo	Opium tincture, stand...	11007213	8
Caelo	Orange flower oil, ar...	13154804	1
Caelo	Orange flower oil, ar...	13154801	1
Caelo	Orange flower oil, ar...		1
Caelo	Orange flower oil, ar...	nachprüfung	1
Caelo	Orange flower oil, ar...	1123005	1
Caelo	Orange flower oil, ar...	11232005	1
Caelo	Orange flower oil, ar...	13121302	1
Caelo	Orange flower water	13096605	3
Caelo	Orange flower water	13057302	2
Caelo	Orange flower water	12359606	3
Caelo	Orange flower water	12328604	3
Caelo	Orange flower water	1235606	1
Caelo	Orange flower water	14156804	1
Caelo	Orange flower water	13339301	1
Caelo	Orange flower water	10371902	1
Caelo	Orange flower water	1339301	1
Caelo	Orange flower water	12032102	1
Caelo	Orange flower water	12328602	1
Caelo	Orange flower water	13339302	2
Caelo	Orange flower water	11327301	2
Caelo	Peanut oil, hydrated	13172801	2
Caelo	Peanut oil, hydrated	13172803	2
Caelo	Peanut oil, hydrated	11266904	1
Caelo	Peanut oil, hydrated	12298204	1
Caelo	Peanut oil, hydrated	12298206	3
Caelo	Peanut oil, hydrated	12298203	1
Caelo	Peppermint spirit 80.2%	11185902	1

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Supplier	Substance	Batch	Spectra
Caelo	Peppermint spirit 80.2%	11339501	1
Caelo	Peppermint spirit 80.2%	12327202	1
Caelo	Peppermint spirit 80.2%	11185901	1
Caelo	Peppermint tincture (...)	24091206	1
Caelo	Peppermint tincture (...)	11207410	1
Caelo	Peppermint tincture (...)	11207414	3
Caelo	Peppermint tincture (...)	12293409	1
Caelo	Peppermint tincture (...)	9089503	1
Caelo	Peppermint tincture (...)	10106507	1
Caelo	Peppermint tincture (...)	9089504	1
Caelo	Plantain herb liquid ...	13008703	2
Caelo	Plantain herb liquid ...	13008706	1
Caelo	Plantain herb liquid ...	11332621	1
Caelo	Propolis tincture (96...	11269521	1
Caelo	Propolis tincture 1.2...	11269511	1
Caelo	Propolis tincture 1.2...	11269516	1
Caelo	Propolis tincture 1.2...	10305414	1
Caelo	Ratanhia tincture (70...	CH:008/0913	1
Caelo	Ratanhia tincture (70...	11204310	1
Caelo	Ratanhia tincture (70...	14101305	1
Caelo	Ratanhia tincture (70...	13051206	5
Caelo	Ratanhia tincture (70...	13051205	1
Caelo	Ratanhia tincture (70...	13051202	1
Caelo	Ratanhia tincture (70...	12255403	2
Caelo	Ratanhia tincture (70...	11292802	5
Caelo	Rose water	12342402	2
Caelo	Rose water	12299802	5
Caelo	Rose water	12299801	2
Caelo	Rose water	12342404	2
Caelo	Rose water	12342406	2
Caelo	Rose water	13137302	2
Caelo	Rose water	12342407	2
Caelo	Rose water	11286005	1
Caelo	Rose water	13137305	6
Caelo	Rose water	1317302	1
Caelo	Rose water	13255902	4
Caelo	Rose water	13306604	6
Caelo	Rose water	15253701	1
Caelo	Rose water	31101305	1
Caelo	Rose water	13137303	1
Caelo	Rose water	12288902	2
Caelo	Rose water	12185405	2
Caelo	Rose water	12123203	1
Caelo	Rose water	11355401	1
Caelo	Rose water	1021301	1
Caelo	Rose water	13306603	3
Caelo	Rose water	12288903	9
Caelo	Rose water	1234201	1
Caelo	Rose water	13343604	2
Caelo	Rose water	12342401	2
Caelo	Rosemary leaf tinctur...	9135005	1
Caelo	Rosemary leaf tinctur...	9135008	1
Caelo	Sage leaf liquid extr...	11372208	1
Caelo	Sage leaf liquid extr...	11372217	1
Caelo	Sage leaf liquid extr...	11372211	2
Caelo	Sage tincture (70%) 1...	9345011	1
Caelo	Sage tincture (70%) 1...	1120912	1
Caelo	Sage tincture (70%) 1...	11220911	1
Caelo	Sage tincture (70%) 1...	14078111	1
Caelo	Sage tincture (70%) 1...	4111M-02476	1

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Supplier	Substance	Batch	Spectra
Caelo	Sage tincture (70%) 1...	13125505	1
Caelo	Sage tincture (70%) 1...	27111308	1
Caelo	Sage tincture (70%) 1...	13125504	1
Caelo	Sage tincture (70%) 1...	10305312	1
Caelo	Sage tincture (70%) 1...	10305316	1
Caelo	Sage tincture (70%) 1...	11220909	1
Caelo	Sage tincture (70%) 1...	12196602	3
Caelo	Sage tincture (70%) 1...	12196607	1
Caelo	Sage tincture (70%) 1...	15081804	1
Caelo	Sage tincture (70%) 1...	12196611	3
Caelo	Siam benzoin tincture...	12228113	1
Caelo	Siam benzoin tincture...	1228119	1
Caelo	Spearmint water	13184501	1
Caelo	Spearmint water	13184503	1
Caelo	St. John's wort oil	13065104	5
Caelo	St. John's wort oil	12293919	2
Caelo	St. John's wort oil	13065105	9
Caelo	St. John's wort oil	15358606	1
Caelo	St. John's wort oil	16037003	1
Caelo	St. John's wort oil	28091204	1
Caelo	St. John's wort oil	4959702	5
Caelo	St. John's wort oil	5346791	1
Caelo	St. John's wort oil	5442802	2
Caelo	St. John's wort oil	15358605	1
Caelo	St. John's wort oil	13065106	5
Caelo	St. John's wort oil	13155802	3
Caelo	St. John's wort oil	13155803	1
Caelo	St. John's wort oil	13252506	1
Caelo	St. John's wort oil	13389218	1
Caelo	St. John's wort oil	14130405	1
Caelo	St. John's wort oil	1501302	1
Caelo	St. John's wort oil	12293918	5
Caelo	St. John's wort oil	11372102	2
Caelo	St. John's wort oil	11205310	1
Caelo	St. John's wort oil	11205309	5
Caelo	St. John's wort oil	11080517	1
Caelo	St. John's wort oil	10380614	1
Caelo	St. John's wort oil	2071201	1
Caelo	St. John's wort oil	2061205	1
Caelo	St. John's wort oil	13155804	8
Caelo	St. John's wort oil	11372104	4
Caelo	St. John's wort oil	12293917	4
Caelo	St. John's wort oil	12293911	8
Caelo	St. John's wort oil	12293903	2
Caelo	St. John's wort oil	12293902	1
Caelo	St. John's wort oil	12292904	1
Caelo	St. John's wort oil	12076904	3
Caelo	St. John's wort oil	12076912	3
Caelo	St. John's wort oil	12076913	8
Caelo	St. John's wort oil	12193404	1
Caelo	St. John's wort tinct...	12237706	1
Caelo	St. John's wort tinct...	122377006	1
Caelo	St. John's wort tinct...	11195217	1
Caelo	St. John's wort tinct...	11195213	1
Caelo	St. John's wort tinct...	11091303	1
Caelo	St. John's wort tinct...	11195216	2
Caelo	St. John's wort tinct...	12237708	1
Caelo	St. John's wort tinct...	12237709	1
Caelo	Standardised cayenne ...	12053902	2
Caelo	Theriac	12067204	1

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Supplier	Substance	Batch	Spectra
Caelo	Theriac	nachprüfung	1
Caelo	Theriac	12067205	1
Caelo	Theriac	1121206	1
Caelo	Theriac	12067201	2
Caelo	Theriac	12067207	2
Caelo	Theriac	11121203	1
Caelo	Theriac	12067214	1
Caelo	Theriac	13187201	3
Caelo	Thyme liquid extract	13036510	1
Caelo	Thyme liquid extract	11090509	2
Caelo	Thyme liquid extract	13036516	1
Caelo	Thyme liquid extract	1313M-01420	1
Caelo	Thyme liquid extract	6838282	1
Caelo	Thyme liquid extract	13036502	2
Caelo	Thyme liquid extract	11090508	1
Caelo	Thyme liquid extract	12072102	2
Caelo	Thyme tincture (70%) ...	10043113	1
Caelo	Thyme tincture (70%) ...	21031311	1
Caelo	Thyme tincture (70%) ...	18101305	1
Caelo	Thyme tincture (70%) ...	18101304	1
Caelo	Thyme tincture (70%) ...	137918	1
Caelo	Thyme tincture (70%) ...	10379108	1
Caelo	Thyme tincture (70%) ...	10379102	1
Caelo	Tormentil tincture (7...	13003018	2
Caelo	Tormentil tincture (7...	12255202	1
Caelo	Tormentil tincture (7...	11278307	2
Caelo	Tormentil tincture (7...	11278310	1
Caelo	Tormentil tincture (7...	13003012	5
Caelo	Tormentil tincture (7...	12255201	1
Caelo	Tormentil tincture (7...	13003002	2
Caelo	Tormentil tincture (7...	614M2484	1
Caelo	Tormentil tincture (7...	11061207	1
Caelo	Tormentil tincture (7...	11278309	1
Caelo	Tormentil tincture (7...	12255204	1
Caelo	Tormentil tincture (7...	13003003	1
Caelo	Tormentil tincture (7...	13003009	3
Caelo	Tormentil tincture (7...	3713Q2484	2
Caelo	Tormentil tincture (7...	13003013	1
Caelo	Tormentil tincture (7...	13263004	1
Caelo	Tormentil tincture (7...	13263007	1
Caelo	Tormentil tincture (7...	1910212484	2
Caelo	Tormentil tincture (7...	2103312484	2
Caelo	Tormentil tincture (7...	3101212484	1
Caelo	Tormentil tincture (7...	13003010	2
Caelo	Tormentil tincture (7...	13003006	1
Caelo	Tormentil tincture (7...	13003008	1
Caelo	Tormentil tincture (7...	11061210	2
Caelo	Tormentil tincture (7...	4212E-02484	1
Caelo	Tormentil tincture (7...	13263003	1
Caelo	Tretinoin solution 3...	11K09-N-03	1
Caelo	Triamcinolone acetoni...	1332501	1
Caelo	Triamcinolone acetoni...	12250701	1
Caelo	Triamcinolone acetoni...	12301201	2
Caelo	Triamcinolone acetoni...	11329001	1
Caelo	Triamcinolone acetoni...	11258801	1
Caelo	Triamcinolone acetoni...	13184701	7
Caelo	Triamcinolone acetoni...	13275801	3
Caelo	Valerian tincture (70...	13003206	6
Caelo	Valerian tincture (70...	13094505-3380319003	1
Caelo	Valerian tincture (70...	11187103	1

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Supplier	Substance	Batch	Spectra
Caelo	Valerian tincture (70...	11379201	3
Caelo	Valerian tincture (70...	11254309	1
Caelo	Valerian tincture (70...	13094505	7
Caelo	Valerian tincture (70...	13184905	4
Caelo	Valerian tincture (70...	18101302	1
Caelo	Valerian tincture (70...	14353011	1
Caelo	Valerian tincture (70...	16030101	1
Caelo	Valerian tincture (70...	11379204	2
Caelo	Valerian tincture (70...	11011308	1
Caelo	Valerian tincture (70...	11379203	2
Caelo	Valerian tincture (70...	8011423	1
Caelo	Valerian tincture (70...	13003205	1
Caelo	Valerian tincture (70...	13052601	1
Caelo	Valerian tincture (70...	13349203	2
Caelo	Valerian tincture (70...	1309505	1
Caelo	Valerian tincture (70...	13094507	5
Caelo	Valerian tincture (70...	13094506	2
Caelo	Valerian tincture (70...	13094503	2
Caelo	Valerian tincture (70...	12294007	4
Caelo	Valerian tincture (70...	12196204	5
Caelo	Valerian tincture (70...	12196203	1
Caelo	Valerian tincture (70...	12113004	3
Caelo	Valerian tincture (70...	12030908	1
Caelo	Valerian tincture (70...	12294002	3
Caelo	Valerian tincture (70...	12294008	2
Caelo	Valerian tincture (70...	12030902	2
Caelo	Valerian tincture (70...	12030904	1
Caelo	Valerian tincture (70...	6099.99.99	1
Caelo	Valerian tincture (70...	12196210	2
Caelo	Valerian tincture (70...	12113002	1
Caelo	Vitamin A-palmitate (...)	12132902	2
Caelo	Vitamin A-palmitate (...)	12132906	4
Caelo	Vitamin A-palmitate (...)	11178101	2
Caelo	Vitamin A-palmitate (...)	11178109	1
Caelo	Vitamin A-palmitate (...)	12132910	5
Caelo	Vitamin A-palmitate (...)	12132904	4
Caelo	Vitamin A-palmitate (...)	12132910	5
Caelo	Vitamin A-palmitate (...)	120404301	2
Caelo	Vitamin A-palmitate (...)	12132904	7
Caelo	Vitamin A-palmitate (...)	13057003	1
Caelo	Vitamin A-palmitate (...)	1013Q-02565	1
Caelo	Vitamin A-palmitate (...)	10316605	1
Caelo	Vitamin A-palmitate (...)	1117801	1
Caelo	Vitamin A-palmitate (...)	12132902	4
Caelo	Vitamin A-palmitate (...)	12132906	4
Caelo	Vitamin A-palmitate (...)	13057002	1
Caelo	Vitamin A-palmitate (...)	3815926	1
Caelo	Vitamin A-palmitate (...)	13296206	1
Caelo	Vitamin A-palmitate (...)	130577002	1
Caelo	Vitamin A-palmitate (...)	130570012132910	1
Caelo	Vitamin A-palmitate (...)	13057002	8
Caelo	Vitamin A-palmitate (...)	1357007	2
Caelo	Vitamin A-palmitate (...)	13296208	1
Caelo	Witch hazel bark liqu...	11165602	1
Caelo	Witch hazel bark liqu...	13044104	2
Caelo	Witch hazel bark liqu...	13044106	1
Caelo	Witch hazel bark liqu...	13044102	3
Caelo	Witch hazel bark liqu...	11165605	1
Caelo	Witch hazel bark water	13324401	1
Caelo	Witch hazel bark water	12376906	2

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Supplier	Substance	Batch	Spectra
Caelo	Witch hazel bark water	12376901	3
Caelo	Witch hazel bark water	13324403	3
Caelo	Witch hazel bark water	12376907	4
Caelo	Witch hazel bark water	11238904	1
Caelo	Witch hazel bark water	12376909	2
Caelo	Witch hazel bark water	12196905	3
Caelo	Witch hazel bark water	14093302	1
Caelo	Witch hazel bark water	12376905	2
Caelo	Witch hazel bark water	12376918	2
Caelo	Witch hazel bark water	11238906	3
Caelo	Witch hazel bark water	15430206	1
Caelo	Witch hazel bark water	12196906	2
Caelo	Witch hazel bark water	13324411	1
Caelo	Witch hazel bark water	12359605	1
Caelo	Witch hazel bark water	11062814	1
Caelo	Witch hazel leaf liqu...	31031404	1
Caelo	Witch hazel leaf liqu...	14112302	1
Caelo	Witch hazel leaf liqu...	16071401	1
Caelo	Witch hazel leaf liqu...	11060505	1
Caelo	Witch hazel leaf liqu...	27081302	1
Caelo	Witch hazel leaf liqu...	12165010	1
Caelo	Witch hazel leaf liqu...	27081303	1
Caelo	Wormwood tincture (70...	11145005	1
Caelo	Wormwood tincture (70...	11145004	1
Caelo	Wormwood tincture (70...	11145001	1
Caelo	Wormwood tincture (70...	12237905	4
Caelo	Wormwood tincture (70...	11145009	1
Caelo	Wormwood tincture (70...	13187404	1
Caelo	Wormwood tincture (70...	12237911	1
Caelo	Wormwood tincture (70...	12237909	4
Caelo	Wormwood tincture (70...	92780419	1
Caelo	Wormwood tincture (70...	10260210	2
Caelo	Wormwood tincture (70...	12237901	1
Caelo	Wormwood tincture (70...	11145008	2
Caelo	Wormwood tincture (70...	11145013	3
Caelo	Wormwood tincture (70...	1114508	1
Caelo	Zinc ointment DAB	13072702	1
Caelo	Zinc ointment DAB	12101302	1
Caelo	Zinc ointment DAB	12098402	4
Caelo	Zinc ointment DAB	13257001	10
Caelo	Zinc ointment DAB	1234602	1
Caelo	Zinc ointment DAB	12042502	1
Caelo	Zinc ointment DAB	7031303	1
Caelo	Zinc ointment DAB	20270912-5	1
Caelo	Zinc ointment DAB	12343602	8
Caelo	Zinc ointment DAB	12042503	2
Caelo	Zinc ointment DAB	11367501	3
Caelo	Zinc ointment DAB	16101202	1
Caelo	Zinc ointment DAB	15003802	1
Caelo	Zinc oxide cream 25% ...	279250	2
Caelo	Zinc oxide cream 25% ...	2795250	1
Caelo	Zinc oxide lotion, aq...	20310812-3	1
Caelo	Zinc oxide lotion, aq...	24101311	1
Caelo	Zinc oxide lotion, aq...	2713M1815	1
Caelo	Zinc oxide lotion, aq...	12309601	7
Caelo	Zinc oxide lotion, aq...	1109779	1
Caelo	Zinc oxide lotion, aq...	12309802	9
Caelo	Zinc oxide lotion, aq...	19041309	1
Caelo	Zinc oxide lotion, aq...	14010502	1
Caelo	Zinc oxide lotion, aq...	28121204	1

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Supplier	Substance	Batch	Spectra
Caelo	Zinc oxide lotion, aq...	14010602	1
Caelo	Zinc oxide lotion, aq...	2713M9101	1
Caelo	Zinc oxide lotion, aq...	3101217039	1
Caelo	Zinc oxide lotion, aq...	15003201	3
Caelo	Zinc oxide lotion, aq...	15061201	1
Caelo	Zinc oxide lotion, aq...	15154301	1
Caelo	Zinc oxide lotion, aq...	15273502	1
Caelo	Zinc oxide lotion, aq...	16003202	1
Caelo	Zinc oxide lotion, aq...	14010501	2
Caelo	Zinc oxide lotion, aq...	13282901	17
Caelo	Zinc oxide lotion, aq...	12211401	10
Caelo	Zinc oxide lotion, aq...	12197103	1
Caelo	Zinc oxide lotion, aq...	12111306	1
Caelo	Zinc oxide lotion, aq...	13087701	19
Caelo	Zinc oxide lotion, aq...	12065401	3
Caelo	Zinc oxide lotion, aq...	13087601	30
Caelo	Zinc oxide lotion, aq...	13283001	3
Caelo	Zinc oxide lotion, aq...	112814101	1
Caelo	Zinc oxide lotion, aq...	11329902	1
Caelo	Zinc oxide lotion, aq...	12065203	1
Caelo	Zinc oxide lotion, aq...	12065301	8
Caelo	Zinc oxide lotion, aq...	13282701	1
Caelo	Zinc oxide lotion, aq...	12309701	5
Caelo	Zinc oxide lotion, aq...	12309702	6
Caelo	Zinc oxide lotion, aq...	13139302	4
Caelo	Zinc oxide lotion, aq...	13139301	19
Caelo	Zinc oxide lotion, aq...	13018801	8
Caelo	Zinc oxide lotion, aq...	1313901	1
Caelo	Zinc oxide lotion, aq...	1230951	1
Caelo	Zinc oxide lotion, aq...	13282801	6
Caelo	Zinc oxide lotion, aq...	1319601	2
Caelo	Zinc oxide lotion, aq...	12211601	2
Caelo	Zinc oxide lotion, aq...	12211701	17
Caelo	Zinc oxide lotion, aq...	12211802	5
Caelo	Zinc oxide lotion, aq...	13139601	33
Caelo	Zinc oxide lotion, aq...	11184501	1
Caelo	Zinc oxide lotion, aq...	1013I-01815	1
Caelo	Zinc oxide lotion, aq...	10082601	1
Caelo	Zinc oxide lotion, aq...	711217039	1
Caelo	Zinc oxide lotion, aq...	12211501	8
Caelo	Zinc oxide lotion, aq...	11184601	1
Caelo	Zinc oxide lotion, aq...	132801	1
Caelo	Zinc oxide lotion, aq...	13024401	6
Caelo	Zinc oxide lotion, aq...	6061301	1
Caelo	Zinc oxide lotion, aq...	4121204	1
Caelo	Zinc oxide lotion, aq...	38112A-01815	1
Caelo	Zinc oxide lotion, aq...	13283103	1
Caelo	Zinc oxide lotion, aq...	13283002	5
Caelo	Zinc oxide lotion, aq...	13018401	18
Caelo	Zinc oxide lotion, aq...	13283101	8
Caelo	Zinc oxide lotion, aq...	11071304	1
Caelo	Zinc oxide lotion, aq...	11071303	1
Caelo	Zinc oxide lotion, aq...	12309501	32
Caelo	Zinc oxide lotion, aq...	13018803	6
Caelo	Zinc oxide oil DAC	12004701	2
Caelo	Zinc oxide oil DAC	13196401	38
Caelo	Zinc oxide oil DAC	2612M-02026	1
Caelo	Zinc oxide oil DAC	12160002	30
Caelo	Zinc oxide oil DAC	12160101	1
Caelo	Zinc oxide oil DAC	13307202	35

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Supplier	Substance	Batch	Spectra
Caelo	Zinc oxide oil DAC	13196501	2
Caelo	Zinc oxide oil DAC	12004601	2
Caelo	Zinc oxide oil DAC	12351702	19
Caelo	Zinc oxide oil DAC	12289801	1
Caelo	Zinc oxide oil DAC	3112M-02026	1
Caelo	Zinc oxide oil DAC	15173002	1
Caelo	Zinc oxide oil DAC	12128602	1
Caelo	Zinc oxide oil DAC	12289802	3
Caelo	Zinc oxide paste SR90	244154	1
Caelo	Zinc oxide paste SR90	271195	1
Caelo	Zinc oxide paste, sof. ...	12366801	1
Caelo	Zinc oxide shaking mi. ...	1308021	1
Caelo	Zinc oxide shaking mi. ...	12261701	1
Caelo	Zinc oxide shaking mi. ...	1324401	1
Caelo	Zinc oxide shaking mi. ...	13244001	1
Caelo	Zinc oxide shaking mi. ...	13080201	3
Caelo	Zinc paste DAB	11290901	1
Caelo	Zinc paste DAB	10345201	3
Caelo	Zinc paste DAB	11321701	4
Caelo	Zinc paste DAB	10245901	2
Caelo	Zinc paste DAB	11364102	2
Caelo	Zinc paste DAB	12066102	1
Caelo	Zinc paste DAB	11321702	1
Caelo	Zinc paste DAB	20271012-1	1
Caelo	Zinc paste DAB	20021310	1
Caelo	Zinc paste DAB	16013302	1
Caelo	Zinc paste DAB	12206401	5
Caelo	Zinc paste DAB	12206501	11
Caelo	Zinc paste DAB	31051302	1
Caelo	Zinc paste DAB	13043301	4
Caelo	Zinc paste DAB	12147801	13
Caelo	Zinc paste DAB	11290801	2
Caelo	Zinc paste DAB	13201701	1
Caelo	Zinc paste DAB	13201801	23
Caelo	Zinc paste DAB	1321903	1
Caelo	Zinc paste DAB	14011402	1
Caelo	Zinc paste DAB	12271702	11
Caelo	Zinc paste DAB	12271601	10
Caelo	Zinc paste DAB	14293401	1
Caelo	Zinc paste DAB	14293302	1
Caelo	Zinc paste DAB	12262301	2
Caelo	Zinc paste DAB	903312054	1
Caelo	Zinc paste DAB	15121-02054	1
Caelo	Zinc paste, soft DAB	3413E-02055	1
Caelo	Zinc paste, soft DAB	12366703	1
Caelo	Zinc paste, soft DAB	12271301	5
Caelo	Zinc paste, soft DAB	12271401	9
Caelo	Zinc paste, soft DAB	14023301	2
Caelo	Zinc paste, soft DAB	12207901	8
Caelo	Zinc paste, soft DAB	13316701	1
Caelo	Zinc paste, soft DAB	12068801	8
Caelo	Zinc paste, soft DAB	11338601	3
Caelo	Zinc paste, soft DAB	11061301	1
Caelo	Zinc paste, soft DAB	13036901	1
Caelo	Zinc paste, soft DAB	12271501	20
Caelo	Zinc paste, soft DAB	711212055	1
Caelo	Zinc paste, soft DAB	70913WZP	1
Caelo	Zinc paste, soft DAB	8081301	1
Caelo	Zinc paste, soft DAB		2
Caelo	Zinc paste, soft DAB	12121501	4

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Supplier	Substance	Batch	Spectra
Caelo	Zinc paste, soft DAB	6021305	1
Caelo	Zinc paste, soft DAB	2713E2055	1
Caelo	Zinc paste, soft DAB	12121601	10
Caelo	Zinc paste, soft DAB	16001201	2
Caelo	Zinc paste, soft DAB	15073001	2
Caelo	Zinc paste, soft DAB	15005202	1
Caelo	Zinc paste, soft DAB	14296801	1
Caelo	Zinc paste, soft DAB	28031401	1
Caelo	Zinc paste, soft DAB	11338801	4
Caelo	Zinc paste, soft DAB	12068701	4
Caelo	Zinc paste, soft DAB	14111313	1
Caelo	Zinc paste, soft DAB	14173001	2
Caelo	Zinc paste, soft DAB	213E-02055	1
Caelo	Zinc paste, soft DAB	14181702	1
Caelo	Zinc paste, soft DAB	14296201	1
Caelo	Zinc paste, soft DAB	1212601	1
Caelo	Zinc paste, soft DAB	414U-02055	1
Caelo	Zinc paste, soft DAB	2101212055	1
Caelo	Zinc paste, soft DAB	13027001	8
Caelo	Zinc paste, soft DAB	1403212055	1
Caelo	Zinc paste, soft DAB	12121302	2
Caelo	Zinc paste, soft DAB	11338401	2
Caelo	Zinc paste, soft DAB	5517500	5
Caelo	Zinc paste, soft DAB	13088602	1
Caelo	Zinc paste, soft DAB	13089101	5
Caelo	Zinc paste, soft DAB	13203701	2
Caelo	Zinc paste, soft DAB	13026901	19
Caelo	Zinc paste, soft DAB	13203301	16
Caelo	Zinc paste, soft DAB	1212401	1
Caelo	Zinc paste, soft DAB	12068901	2
Caelo	Zinc paste, soft DAB	13004101	1
Caelo	Zinc paste, soft DAB	13088701	29
Caelo	Zinc paste, soft DAB	14023801	1
Caelo	Zinc paste, soft DAB	14023701	2
Caelo	Zinc paste, soft DAB	11099003	1
Caelo	Zinc paste, soft DAB	13316601	5
Caelo	Zinc paste, soft DAB	13387801	8
Caelo	Zinc paste, soft DAB	11202101	1
Caelo	Zinc paste, soft DAB	11338001	2
Caelo	Zinc paste, soft DAB	11269701	2
Caelo	Zinc paste, soft DAB	208212055	1
Caelo	Zinc paste, soft DAB	13089001	15
Caelo	Zinc paste, soft DAB	13088901	12
Caelo	Zinc paste, soft DAB	13088801	10
Caelo	Zinc paste, soft DAB	12069001	5
Caelo	Zinc paste, soft DAB	12207801	1
Caelo	Zinc paste, soft DAB	12366701	11
Caelo	Zinc paste, soft DAB	12308307	1
Caelo	Zinc paste, soft DAB	13026702	5
Caelo	Zinc paste, soft DAB	17111203	1
Caelo	Zinc paste, soft DAB	5611900	3
Caelo	Zinc paste, soft DAB	12208201	16
Caelo	Zinc paste, soft DAB	12121401	7
Caelo	Zinc paste, soft DAB	12366801	11
Caelo	Zinc paste, soft DAB	12208101	6
Caelo	Zinc paste, soft DAB	63075606	1
Caelo	Zinc paste, soft DAB	91107159	1
Caelo	Zinc paste, soft DAB	1601312055	1
Caelo	Zinc paste, soft DAB	13040201	9
Caelo	Zinc paste, soft DAB	13026801	7

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Supplier	Substance	Batch	Spectra
Caelo	Zinc paste, soft DAB	13316301	16
Caelo	Zinc paste, soft DAB	13203501	9
Caelo	Zinc paste, soft DAB	13203401	9
Caelo	Zinc paste, soft DAB	13088/01	1
Caelo	Zinc paste, soft DAB	14117801	1
Caelo	Zinc paste, soft DAB	13316401	5
Caelo	Zinc paste, soft DAB	13388001	2
Caelo	Zinc paste, soft DAB	1268901	1
Caelo	Zinc paste, soft DAB	13316501	6
Caelo	Zinc paste, soft DRF ...	13094201	2
Caelo	Zinc paste, soft DRF ...	12160302	1
Caesar & Loretz	Plantain herb liquid ...	13008704	2
Caesar & Loretz GmbH	Coal tar solution	72816068	1
Caesar & Loretz GmbH	Hydrophobic triclosan...	S041303.1	3
Caesar & Loretz GmbH	Matricaria oil, fat	12189803	2
Caesar & Loretz GmbH	Matricaria oil, fat	13204304	2
Caesar & Loretz GmbH	Vitamin A-palmitate (...)	10316605	1
Caesar & Loretz GmbH	Zinc oxide lotion, aq. ...	13405901	4
Caesar & Loretz GmbH	Zinc paste DAB	281972	1
Caesar & Loretz GmbH ...	Zinc paste, soft DAB	11269601	2
Caesar & Loretz GmbH, ...	Benzalkonium chloride	12033407	2
Caesar & Loretz/ Noweda	Hydroxyethylcellulose...	5B150213	1
Caesar & Loretz/ Noweda	Plantain herb liquid ...	11332616	3
Caesar & Loretz/ Noweda	Plantain herb liquid ...	11332613	2
Caesar & Loretz/ Noweda	Plantain herb liquid ...	11332620	1
Caesar & Loretz/ Noweda	Plantain herb liquid ...	11332611	1
Caesar & Loretz/ Noweda	Plantain herb liquid ...	13008708	2
Caesar § Lorenz GmbH	Aloe vera oil (with a...	12383707	1
Caesar&Loretz GmbH/An...	Peppermint spirit 80.2%	13252802	1
Caesar&lorenz,Phoenix	Lard	11095310	1
Caesar/Noweda	Gentian tincture (70%...	13036408	1
Caesar/Noweda	Ratanhia tincture (70...	13051210	1
Calo	Zinc oxide lotion, aq. ...	14211601	1
Cheplapharm Arzneimit...	Valerian tincture (70...	70713	1
Defektur	Hydrogen peroxide sol...	6629	1
Defektur	Hydrogen peroxide sol...	6935	1
Defektur	Hydrogen peroxide sol...	6726	1
Defektur	Hydrophilic metronida...	35121-07001	1
Defektur	Hydrophilic metronida...	4612E-03387	1
Defektur	Hydrophilic metronida...	4812E-07001	1
Defektur	Hydrophilic metronida...	1813Q-07001	1
Defektur	Hydrophilic metronida...	3412M-07001	1
Defektur	Hydrophilic metronida...	4912Q-07001	1
Defektur	Hydrophilic metronida...	3212M-03387	1
Defektur	Hydrophilic metronida...	813A-07001	1
Defektur	Hydrophilic metronida...	2713E-07001	1
Defektur	Hydrophilic metronida...	1613a-07001	1
Defektur	Hydrophilic metronida...	1913A-07001	1
Defektur	Hydrophilic metronida...	1813E-07001	1
Defektur	Hydrophilic metronida...	4112E-07001	1
Defektur	Hydrophilic metronida...	4012A-07001	1
Defektur	Hydrophilic metronida...	3712Q-07001	1
Defektur	Hydrophilic metronida...	2513q-07001	1
Defektur	Oxytetracycline ointm...	43/13	1
Defektur	Oxytetracycline ointm...	41/13	1
Defektur	Oxytetracycline ointm...	49/12	1
Defektur	Oxytetracycline ointm...	8/13	1
Defektur	Oxytetracycline ointm...	25/13	1
Defektur	Oxytetracycline ointm...	55/12	1
Defektur	Oxytetracycline ointm...	50/13	1

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Supplier	Substance	Batch	Spectra
Defektur	Oxytetracycline ointm. ...	12/13	1
Defektur	Triamcinolone acetoni. ...	3813Q	1
Defektur	Triamcinolone acetoni. ...	4213E	1
Defektur	Triamcinolone acetoni. ...	4713A	1
Defektur	Triamcinolone acetoni. ...	4913Q	1
Defektur	Zinc paste, soft DAB	11/13	1
Defektur	Zinc paste, soft DAB	54/12	1
Defektur	Zinc paste, soft DAB	32/13	1
Defektur	Zinc paste, soft DAB	56/13	1
Eigenherstellung	Hydrophilic metronida. ...	912Q-07001	1
Eigenherstellung	Opium tincture, stand. ...	70613PML01	2
Erika apotheke	Gentian tincture (70%. ...	1122504	1
Erika apotheke	Tormentil tincture (7. ...	13003001	1
Erika apotheke	Wormwood tincture (70. ...	12237906	1
Erika Apotheke	Orange flower water	12359601	1
Erika Apotheke	Wormwood tincture (70. ...	12237902	3
Erika Apotheke	Wormwood tincture (70. ...	313E-07062	1
EuRho	Castor oil, hydrated	1212008-01	1
EuRho	Valerian tincture (70. ...	1301003-01	1
EuRho/Phönix	Castor oil, hydrated	1412006-01	1
Euro OTC	Arnica tincture (70%). ...	1306038-01	1
Euro OTC	Arnica tincture (70%). ...	1112029-01	1
Euro OTC	Campher oil 10%	15338204	1
Euro OTC	Castor oil, hydrated	1109001-01	2
Euro OTC	Castor oil, hydrated	1910212009	1
Euro OTC	Castor oil, hydrated	1512212009	1
Euro OTC	Castor oil, hydrated	1412006-02	1
Euro OTC	Castor oil, hydrated	1206039-02	2
Euro OTC	Castor oil, hydrated	1206039-01	2
Euro OTC	Castor oil, hydrated	1202041-02	1
Euro OTC	Castor oil, hydrated	2507213553	1
Euro OTC	Castor oil, hydrated	1112002-02	1
Euro OTC	Castor oil, hydrated	120204-01	1
Euro OTC	Coal tar solution	1110031-01	6
Euro OTC	Coal tar solution	1110031	1
Euro OTC	Coal tar solution	1110031-02	6
Euro OTC	Coal tar solution	1307027-01	2
Euro OTC	Tretinoin solution 3. ...	13c28-n01	1
Euro OTC	Valerian tincture (70. ...	1304041-01	1
Euro OTC	Vitamin A-palmitate (...)	1305003-01	2
Euro OTC	Vitamin A-palmitate (...)	1305003-01-342631115	1
Euro OTC	Vitamin A-palmitate (...)	1204043-01	3
Euro OTC	Vitamin A-palmitate (...)	1204043-01	4
Euro OTC	Vitamin A-palmitate (...)	1310030-01	1
Euro OTC	Zinc paste, soft DAB	1009043-01	3
Euro OTC	Zinc paste, soft DAB	1211014-01	8
Euro OTC	Zinc paste, soft DAB	121014-01	1
Euro OTC	Zinc paste, soft DAB	121101401	1
Euro OTC	Zinc paste, soft DAB	1108059-01	4
Euro OTC	Zinc paste, soft DAB	1310019-01	2
Euro OTC	Zinc paste, soft DAB	214I-02055	1
Euro OTC	Zinc paste, soft DAB	13211014-01	1
EUro/AHD	Vitamin A-palmitate (...)	1211032-01	2
Fagron	Carbomer gel 1%	1302D002	7
Fagron	Carbomer gel 1%	1309D002	1
Fagron	Carbomer gel 1%	1309D001	1
Fagron	Carbomer gel 1%	1211D010	2
Fagron	Castor oil, hydrated	10L02-N03	1
Fagron	Coal tar solution	12H28-N05	1
Fagron	Coal tar solution	11/05-N12	1

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Supplier	Substance	Batch	Spectra
Fagron	Coal tar solution	12L05-N02	4
Fagron	Coal tar solution	11-05-N12	1
Fagron	Coal tar solution	4513E1799	1
Fagron	Coal tar solution	2011.07.0288	2
Fagron	Coal tar solution	18061301	1
Fagron	Coal tar solution	11F21-N01	3
Fagron	Coal tar solution	13H06N02	1
Fagron	Coal tar solution	13H06-N02	10
Fagron	Coal tar solution	12F19-N08	4
Fagron	Coal tar solution	12E08-N08	1
Fagron	Coal tar solution	20230712-6	1
Fagron	Coal tar solution	13I26-N02	1
Fagron	Hydrogen peroxide sol...	13G09-M07	1
Fagron	Hydrogen peroxide sol...	12I06-M05	1
Fagron	Hydrogen peroxide sol...	13A02-M10	1
Fagron	Hydrogen peroxide sol...	13A02-M13	1
Fagron	Hydrogen peroxide sol...	13D05-M04	1
Fagron	Hydrogen peroxide sol...	13G09-M03	1
Fagron	Hydrogen peroxide sol...	13K07-M04	1
Fagron	Hydrogen peroxide sol...	13G12-M09	1
Fagron	Hydrogen peroxide sol...	13G12-M06	1
Fagron	Hydroxyethylcellulose...	13009401	3
Fagron	Hydroxyethylcellulose...	12351401	1
Fagron	Iodine tincture	11309402	1
Fagron	Methylrosanilinium ch...	12D19-N01	1
Fagron	Opium tincture, stand...	9006012/Maros	1
Fagron	Opium tincture, stand...	5007714	2
Fagron	Rose water	12H20-N09	4
Fagron	Rose water	12H-20-N09	1
Fagron	Rose water	13B01-N01	1
Fagron	St. John's wort oil	13A30-N09	1
Fagron	St. John's wort oil	5346701	6
Fagron	St. John's wort oil	12A30-N09	1
Fagron	St. John's wort oil	12L17-N15	1
Fagron	Tretinoin solution 3...	1308D00213/11-N04	1
Fagron	Tretinoin solution 3...	1308D002	1
Fagron	Tretinoin solution 3...	13C25-N01	1
Fagron	Tretinoin solution 3...	13C28-N01	4
Fagron	Tretinoin solution 3...	13I11-N04	4
Fagron	Tretinoin solution 3...	19061306	1
Fagron	Tretinoin solution 3...	1108D001	1
Fagron	Tretinoin solution 3...	1204D004	1
Fagron	Tretinoin solution 3...	12C08-N14	4
Fagron	Tretinoin solution 3...	13/11-N04	1
Fagron	Triamcinolone acetoni...	214Q	1
Fagron	Vitamin A-palmitate (...)	13C19-N12	3
Fagron	Wormwood tincture (70...	13187402	1
Fagron	Zinc oxide lotion, aq...	13K19-T02-014523	1
Fagron	Zinc oxide lotion, aq...	4213Q-01815	1
Fagron	Zinc oxide lotion, aq...	10H19-T01-000747	1
Fagron	Zinc oxide oil SR 90	n.Anbruch3Monate	1
Fagron	Zinc paste DAB	12I06-T01	1
Fagron	Zinc paste DAB	9k06-t02	1
Fagron	Zinc paste, soft DAB	4113A-02055	1
Fagron	Zinc paste, soft DAB	12271502	5
Fagron	Zinc paste, soft DAB	10D15-T01	1
Fagron	Zinc paste, soft DAB	12/26-T03	1
Fagron	Zinc paste, soft DAB	12J26-T03	6
Fagron	Zinc paste, soft DAB	13H13-T05-006158	1
Fiebig	Coal tar solution	9345501	3

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Supplier	Substance	Batch	Spectra
Fiebig	Hydrogen peroxide sol. . .	61007B	7
Fiebig	Zinc paste DAB	268489	1
Fiebig 23.10.12 ek:6, . . .	Theriac	12067202	1
Fiebig ek:5.69EUR 10.08. . .	Witch hazel bark water	11238911	2
Finze	Zinc oxide lotion, aq. . .	12065501	5
Fischar	Hydrogen peroxide sol. . .	631109	1
Fischar	Hydrogen peroxide sol. . .	6311092	2
Fischar	Hydrogen peroxide sol. . .	6312061	1
Fischar	Hydrogen peroxide sol. . .	6315084	1
Fischar	Hydrogen peroxide sol. . .	6312073	2
Fischar	Hydrogen peroxide sol. . .	6312082	1
Fischar	Hydrogen peroxide sol. . .	6312077	2
Fischar	Hydrogen peroxide sol. . .	6312081	3
Fischar	Hydrogen peroxide sol. . .	6313025	2
Fischar	Hydrogen peroxide sol. . .	6313061	4
Fischar/AHD	Hydrogen peroxide sol. . .	6313062	1
Fischar/Anzag	Hydrogen peroxide sol. . .	6313064	1
Fischar/G	Hydrogen peroxide sol. . .	6313033	1
Fischar/G	Hydrogen peroxide sol. . .	6313093	2
Fischar/G	Hydrogen peroxide sol. . .	6312072	1
Fischar/Gehe	Hydrogen peroxide sol. . .	6313102	1
Fischar/GEHE/16.04.2013	Hydrogen peroxide sol. . .	6312114	3
Fischar/GUMO /02.08.2. . .	Hydrogen peroxide sol. . .	6313027	6
Fischar/Sanacorp	Hydrogen peroxide sol. . .	6312111	1
Fischbar	Hydrogen peroxide sol. . .	4101202	1
Gehe	Bitter orange peel ti. . .	11187211	1
Gehe	Castor oil, hydrated	272591	4
Gehe	Coal tar solution	701972-0001	2
Gehe	Coal tar solution	12A20-N04	1
Gehe	Hydrogen peroxide sol. . .	6314021	2
Gehe	Hydrogen peroxide sol. . .	6312074	4
Gehe	Hydrophilic metronida. . .	5513E-03387	1
Gehe	Hydrophilic metronida. . .	5112Q-07001	1
Gehe	Hydrophilic metronida. . .	4813E-07001	1
Gehe	Hydrophilic metronida. . .	3613E-07001	1
Gehe	Hydrophilic metronida. . .	2512Q-07001	2
Gehe	Hydrophilic metronida. . .	1213E-07001	2
Gehe	Hydrophilic metronida. . .	1013Q-07001	1
Gehe	Hydrophilic metronida. . .	114M-07001	1
Gehe	Hydrophilic metronida. . .	2813M-07001	1
Gehe	Hydrophobic triclosan. . .	S091107.1	2
Gehe	Hydrophobic triclosan. . .	S031103.1	1
Gehe	Hydrophobic triclosan. . .	S101209.1	14
Gehe	Hydrophobic triclosan. . .	S021201.1	5
Gehe	Hydroxyethylcellulose. . .	22b070912	1
Gehe	Hydroxyethylcellulose. . .	5B090312	4
Gehe	Methoxsalen 0.006% Co. . .	13D004A	1
Gehe	Methoxsalen 0.006% Co. . .	13D004B	1
Gehe	Metronidazole 10% (no. . .	8B170712	1
Gehe	Metronidazole 10% (no. . .	4B170413	1
Gehe	Opium tincture, stand. . .	6007814	2
Gehe	Searing paste SR	10B030712	1
Gehe	Searing paste SR	4B080313	1
Gehe	Vitamin A-palmitate (. . .	1110018-01	2
Gehe	Vitamin A-palmitate (. . .	1211032-01	4
Gehe	Vitamin A-palmitate (. . .	11178103	2
Gehe	Vitamin A-palmitate (. . .	11178101	3
Gehe	Zinc oxide lotion, aq. . .	12211402	7
Gehe	Zinc oxide oil DAC	275086	1
Gehe	Zinc oxide oil DAC	279563	3

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Supplier	Substance	Batch	Spectra
Gehe	Zinc oxide oil DAC	282085	1
Gehe	Zinc oxide oil DAC	289826	1
Gehe	Zinc oxide oil DAC	275085	1
Gehe	Zinc oxide paste SR90	279386	1
Gehe	Zinc oxide paste SR90	276199	2
Gehe	Zinc oxide paste SR90	270919	1
Gehe	Zinc oxide paste SR90	268240	1
Gehe	Zinc oxide paste SR90	266451	1
Gehe	Zinc oxide paste SR90	264198	1
Gehe	Zinc oxide paste, sof. ...	36B231012	1
Gehe	Zinc oxide paste, sof. ...	23B160713	1
Gehe	Zinc oxide paste, sof. ...	260912	1
Gehe	Zinc oxide paste, sof. ...	30071502	1
Gehe	Zinc paste DAB	276144	3
Gehe	Zinc paste DAB	271138	3
Gehe	Zinc paste, soft DAB	1B110112	1
Gehe	Zinc paste, soft DAB	130112	1
Gehe	Zinc paste, soft DAB	270462	1
Gehe	Zinc paste, soft DAB	12A250412	1
GEHE	Hydrogen peroxide sol. ...		14
GEHE	Hydrogen peroxide sol. ...	H216091/1	1
Gehe 06.08.2013	Hydrogen peroxide sol. ...	6312065	1
Gehe 06.09.13	Rosemary leaf tinctur. ...	11323611	1
gehe 11.06.2013	Zinc paste DAB	276141	2
gehe 11.06.2013	Zinc paste, soft DAB	12D10-T03	1
Gehe 12.04.2013	Lime water	12177901	1
Gehe 16.04.2013	Coconut oil, hardened	13010803	1
Gehe 16.05.2013	Comfrey root tincture. ...	12054016	2
Gehe 26.09.13	Wormwood tincture (70. ...	12237913	2
Gehe/Fischar/11.12.2012	Hydrogen peroxide sol. ...	6312105	8
GEHE/Fischar/12.06.2012	Hydrogen peroxide sol. ...	6312012	3
Gehe/Fischar11.07.2012	Hydrogen peroxide sol. ...	6312051	9
Gehe/Maros	Opium tincture, stand. ...	11006112	15
Gehrlicher	Pansy mother tincture	RU1775	1
Gehrlicher/Gehrlicher	Burnet root mother ti. ...	U3600	1
Großhandel	Arnica tincture (70%). ...	1211003-01	5
Großhandel	Arnica tincture (70%). ...	1204046-01	4
Großhandel	Coal tar solution	111031-01	1
Großhandel	Matricaria flower tin. ...	11269920	4
Großhandel	Sage tincture (70%) 1. ...	11220912	1
Großhandel	Sage tincture (70%) 1. ...	12196612	4
Großhandel	Vitamin A-palmitate (...)	13057007	4
Großhandel	Zinc oxide lotion, aq. ...	13087501	12
Großhandel	Zinc paste DAB	13043502	4
Großhandel	Zinc paste DAB	12147903	2
H.Lamotte/Noweda	Castor oil, hydrated	123384	1
Hanosan	Strophanthus seed mot. ...	316899	1
Hanosan	Strophanthus seed mot. ...	348059	1
Hedinger	Hydrogen peroxide sol. ...	301207	1
Hedinger	Hydrogen peroxide sol. ...	301210	1
Hedinger	Hydrogen peroxide sol. ...	301212	1
Hedinger	Hydrogen peroxide sol. ...	301208	1
Hedinger	Hydrogen peroxide sol. ...	301205	1
Hedinger	Hydrogen peroxide sol. ...	301211	1
Hedinger	Hydrogen peroxide sol. ...	610108	1
Hedinger	Hydrogen peroxide sol. ...	61008b	1
Hedinger	Hydrogen peroxide sol. ...	61006B	2
Hedinger	Hydrogen peroxide sol. ...	61005B	3
Hedinger	Hydrogen peroxide sol. ...	61010b	2
Hedinger	Hydrogen peroxide sol. ...	8111302	1

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Supplier	Substance	Batch	Spectra
Hedinger	Hydrogen peroxide sol. ...	210913H202	1
Hedinger	Hydrogen peroxide sol. ...	610128	1
Hedinger	Hydrogen peroxide sol. ...	61011b	2
Hedinger	Witch hazel bark water	20153B	2
Hedinger / Gehe	Hydrogen peroxide sol. ...	(061b)061b	2
Hedinger / Gehe	Hydrogen peroxide sol. ...	64044B	1
Hedinger / Sanacorp	Sodium hypochlorite s. ...	46386	1
Hedinger Jenne	Hydrogen peroxide sol. ...	61009B	24
Hedinger Jenne	Hydrogen peroxide sol. ...	61011B	28
Hedinger/ Gehe	Sodium hypochlorite s. ...	46375	1
Hedinger/ Phönix	Sodium hypochlorite s. ...	46392	1
Hedinger/AHD	Hydrogen peroxide sol. ...	61010B	1
Hedinger/AHD	Hydrogen peroxide sol. ...	61012B	6
Hedinger/AHD	Hydrogen peroxide sol. ...	61010B	23
Hedinger/Anzag	Hydrogen peroxide sol. ...	4413A-01720	1
Hedinger/Anzag 21.07....	Hydrogen peroxide sol. ...	61008B	21
Henry Lamotte	Zinc oxide lotion, aq. ...	60480	1
Henry Lamotte GmbH/Ho. ...	Zinc oxide lotion, aq. ...	5289300	3
henry lamotte oils gmbh	Zinc oxide lotion, aq. ...	90616-1	1
henry lamotte oils gmbh	Zinc oxide lotion, aq. ...	6000083002	1
henry lamotte oils gmbh	Zinc oxide lotion, aq. ...	5735500	1
Henry Lamotte Oils GmbH	Zinc oxide lotion, aq. ...	600320602	1
Henry Lamotte Oils GmbH	Zinc paste, soft DAB	5316600	8
Henry Lamotte Oils Gm. ...	Zinc paste, soft DAB	5375700	4
Henry Lamotte Oils, A. ...	Zinc oxide lotion, aq. ...	5375600	12
Henry Lamotte/ 24.04....	Zinc oxide lotion, aq. ...	1221401	2
HenryLamotte/Sanacorp	St. John's wort oil	5308402-3457312120	1
Herbeta Arzneimittel	Hydrogen peroxide sol. ...	15061202	1
Herstellung	Hydrogen peroxide sol. ...	6313072	1
Hetterich/Teofarma	Myrrh tincture (90%) ...	139101	1
Holdermann/Lamotte	Castor oil, hydrated	5280301	2
Hustadt Apotheke	Hydroxyethylcellulose...	12128101	1
Hustadt Apotheke	Ratanhia tincture (70. ...	12255401	7
ichthyol	Clobetasol 0.5% Corde. ...	5112M-03390	1
ichthyol	Clobetasol 0.5% Corde. ...	1713M-03390	1
Ichthyol	Betamethason-V 1.22% ...	110001	1
Ichthyol	Clobetasol 0.5% Corde. ...	11D003	7
Ichthyol	Clobetasol 0.5% Corde. ...	10D024	1
Ichthyol	Clobetasol 0.5% Corde. ...	12d012	1
Ichthyol	Methoxsalen 0.006% Co. ...	130004	2
Ichthyol	Methoxsalen 0.006% Co. ...	14D001	1
Ichthyol- Gesellschaft	Methoxsalen 0.006% Co. ...	13D013	7
Ichthyol Gesellschaft. ...	Clobetasol 0.5% Corde. ...	11D034	6
ICHTHYOL/ahp	Methoxsalen 0.006% Co. ...	13d004	1
Ichthyol/Gehe	Methoxsalen 0.006% Co. ...	13D004	28
Ichthyol/Jenne	Betamethason-V 1.22% ...	12D015	10
Ichthyol/Jenne	Betamethason-V 1.22% ...	12D015	2
Ichthyol/Noweda	Betamethason-V 1.22% ...	120015	1
Ichthyol-Gesellschaft. ...	Betamethason-V 1.22% ...	11D001	3
Ichthyol-Gesellschaft. ...	Gentamicin 1% Cordes® ...	9D002	1
Ichtyol	Clobetasol 0.5% Corde. ...	12D012	7
Infectopham/Gehe	Hydrophobic triclosan...	S021201.	1
infectopharm	Hydrophobic triclosan...	s101209.1	1
infectopharm	Hydrophobic triclosan...	S041302.1	2
Infectopharm	Hydrophobic triclosan...	S031101.1	1
Infectopharm	Hydrophobic triclosan...	20160712-1	1
Infectopharm	Hydrophobic triclosan...	S091203.1	7
Infectopharm	Hydrophobic triclosan...	S04131011	1
Infectopharm	Hydrophobic triclosan...	s1012091	1
Infectopharm	Hydrophobic triclosan...	S101208.1	13

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Supplier	Substance	Batch	Spectra
Infectopharm	Hydrophobic triclosan...	S101207.1	10
Infectopharm	Hydrophobic triclosan...	S091109.1	2
Infectopharm	Hydrophobic triclosan...	S041301.1	7
Infectopharm	Hydrophobic triclosan...	S031502.1	1
Infectopharm	Hydrophobic triclosan...	S0212041	1
InfectoPharm	Hydrophobic triclosan...	S091103.1	3
InfectoPharm / 04.09...	Hydrophobic triclosan...	S091104.1	1
InfectoPharm / Gehe	Hydrophobic triclosan...	S0413041	1
Infectopharm, Noweda	Hydrophobic triclosan...	S021203.1	4
Infectopharm, Noweda	Hydrophobic triclosan...	S0231204.1	1
Infectopharm,AHC	Hydrophobic triclosan...	S101304.1	1
Infectopharm/AHD	Hydrophobic triclosan...	S1012209.1	1
InfectoPharm/GEHE	Hydrophobic triclosan...	S.091203.1	1
infectopharm/Noweda	Hydrophobic triclosan...	S041301.1	4
Infectopharm/Noweda	Hydrophobic triclosan...	S0413011	1
InfectoPharm/Phoenix	Hydrophobic triclosan...	S021201.1	4
InfectoPharm/Phönix	Hydrophobic triclosan...	1101410005	1
Jenne	Myrrh tincture (90%) ...	12197205	5
Kehr	Zinc ointment DAB	274127	2
Kehr	Zinc ointment DAB	272144	1
Kehr	Zinc oxide lotion, aq. ...	12065202	2
Klenk	Calendula oil, fat	12308503	2
Krieger	Coal tar solution	11319212	3
labor	Hydrogen peroxide sol...	7571	1
Labor	Hydrogen peroxide sol...	7798	1
Labor	Hydrogen peroxide sol...	8698	1
Labor	Hydrogen peroxide sol...	7408	1
Labor	Hydrogen peroxide sol...	9848	1
Labor	Hydrogen peroxide sol...	7143	1
Labor	Hydrogen peroxide sol...	7991	1
Labor	Hydrogen peroxide sol...	7926	1
Labor	Hydrogen peroxide sol...	7799	1
Labor	Hydrogen peroxide sol...	9757	1
Labor	Hydrogen peroxide sol...	9266	1
Labor	Hydrogen peroxide sol...	9020	1
Labor	Hydrogen peroxide sol...	9634	1
Labor	Hydrogen peroxide sol...	8762	1
Labor	Hydrogen peroxide sol...	9758	1
Labor	Hydrogen peroxide sol...	9957	1
lamotte	Castor oil, hydrated	5188401	2
lamotte	Zinc oxide lotion, aq. ...	6003206002	2
Lamotte	Arnica tincture (70%)...	5139400	1
Lamotte	St. John's wort oil	5346702	14
Lamotte	Zinc oxide lotion, aq. ...	60460	1
Lamotte	Zinc oxide lotion, aq. ...	5651500	1
Lamotte	Zinc oxide lotion, aq. ...	5216200	1
Lamotte	Zinc oxide lotion, aq. ...	5099300	1
Lamotte	Zinc oxide lotion, aq. ...	5163600	2
Lamotte	Zinc paste, soft DAB	5216300	4
Lamotte / Gehe	Castor oil, hydrated	5138701	3
Lamotte / Gehe	Zinc oxide lotion, aq. ...	5517400	12
Lamotte / Gehe	Zinc oxide lotion, aq. ...	5321300	10
Lamotte / Sanacorp	St. John's wort oil	517601	1
Lamotte Sanacorp	St. John's wort oil	5308402	3
Lamotte/ Finze	Zinc oxide lotion, aq. ...	5563300	2
lamotte/Noweda	Zinc paste, soft DAB	5447900	4
Leyhs/Noweda	Methylrosanilinium ch...	124141	1
Maros	Angelica root tinctur...	1028713	2
Maros	Angelica root tinctur...	8030113	1
Maros	Bitter candytuft fres...	5408	1

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Supplier	Substance	Batch	Spectra
Maros	Bitter candytuft fres...	5433	1
Maros	Marian thistle fruit ...	U3762	2
Maros	Matricaria liquid ext...	6990	3
Maros	Melissa leaf liquid e...	6399	3
Maros	Opium tincture, stand...	6006713	29
Maros	Opium tincture, stand...	13071303	1
Maros	Opium tincture, stand...	1006313	12
Maros	Opium tincture, stand...	2004511	1
Maros	Opium tincture, stand...	15031302	1
Maros	Opium tincture, stand...	4005612	4
Maros	Opium tincture, stand...	8005812	5
Maros	Opium tincture, stand...	9006012	16
Maros	Peppermint leaf mothe...	RU2432	2
Maros	Peppermint tincture (...)	RU2432	1
Maros	St. John's wort oil	9758	1
Maros	St. John's wort oil	97583x	1
Maros	Thyme liquid extract	1156	1
Maros Arznei GmbH	Opium tincture, stand...	8006913	23
Maros Arznei GmbH	Opium tincture, stand...	4006513	32
Maros Arznei GmbH	Opium tincture, stand...	11007113	7
MAROS Arznei GmbH	Opium tincture, stand...	7006813	16
Maros Arznei GmbH/Anzag	Opium tincture, stand...	2005412	1
Maros/direkt/07.05.13	Strophanthus seed mot...	4029013	1
Maros/direkt/15.01.14	Strophanthus seed mot...	1031014	3
Maros/direkt/16.08.13	Strophanthus seed mot...	8029813	1
Maros/direkt/21.10.13	Strophanthus seed mot...	10030413	2
Maros/direkt/28.02.14	Strophanthus seed mot...	2031214	5
Maros/Maros	Cistus tincture 1:5	11027812	1
Maros/Maros	Strophanthus seed mot...	6029813	2
Maros/Phoenix	Opium tincture, stand...	60066713	1
müller	Propolis tincture 1.2...	131206	1
Nachprüfung	Chinese cinnamon oil		1
Nachprüfung	Gentian tincture (70%...	411E02442	1
Nachprüfung	Standardised cayenne ...	2413M-03232	1
noweda	Witch hazel bark water	12100302	1
Noweda	Arnica tincture (70%)...	1106037-01	1
Noweda	Betamethason-V 1.22% ...	11D035	10
Noweda	Castor oil, hydrated	12114603	4
Noweda	Castor oil, hydrated	268877	2
Noweda	Coal tar solution	11319204	10
Noweda	Gentamicin 1% Cordes®...	12D010	6
Noweda	Gentamicin 1% Cordes®...	10D026	6
Noweda	Methoxsalen 0.006% Co...	12D011	8
Noweda	Methoxsalen 0.006% Co...	11D006	1
Noweda	Myrrh tincture (90%) ...	1219104	1
Noweda	Opium tincture, stand...	1106112	2
Noweda	Orange flower oil, ar...	10267805	1
Noweda	Ratanhia tincture (70...	12255406	1
Noweda	Thyme liquid extract	10198605	1
Noweda	Tretinoin solution 3...	12G05-N15	5
Noweda	Triamcinolone acetoni...	12080701	1
Noweda	Triamcinolone acetoni...	11359001	1
Noweda	Vitamin A-palmitate (...)	13C19-N12	1
Noweda	Vitamin A-palmitate (...)	13F26-N08	5
Noweda	Witch hazel bark water	11062805	1
Noweda	Witch hazel leaf liqu...	12095405	1
Noweda	Zinc ointment DAB	11271001	3
Noweda	Zinc oxide lotion, aq...	11281401	2
Noweda	Zinc oxide lotion, aq...	11329903	3
Noweda	Zinc oxide lotion, aq...	1211701	1

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Supplier	Substance	Batch	Spectra
Noweda	Zinc paste DAB	276606	1
Noweda	Zinc paste, soft DAB	11338501	3
Noweda	Zinc paste, soft DAB	1138601	1
Noweda/apomix	Clobatesol propionate...	13A131113	1
Noweda/Fischar	Hydrogen peroxide sol...	6313075	2
Noweda/Fischar	Hydrogen peroxide sol...	6313024	1
Noweda/Fischar	Hydrogen peroxide sol...	6313052	1
Noweda/Lamotte	Zinc oxide lotion, aq...	5447800	9
Otto Fischar	Hydrogen peroxide sol...	6313101	1
Otto Fischar / Noweda	Hydrogen peroxide sol...	6314011	1
Otto Fischar gmbh	Hydrogen peroxide sol...	6314113	1
Otto Fischar gmbh	Hydrogen peroxide sol...	6315031	1
Otto Fischar GmbH	Hydrogen peroxide sol...	6312021	3
Otto Fischar GmbH	Rose water	5354081	1
Otto Fischar GmbH & C...	Lactic acid 80% L(+)	20020271	1
Otto Fischar GmbH& Co...	Hydrogen peroxide sol...	6313055	5
Park Apotheke	Matricaria flower tin...	nachprüfung	1
pharmachem	Zinc oxide oil DAC	90512	1
pharmachem	Zinc oxide paste, sof...	211112	1
Pharmachem	Oxytetracycline ointm...	230113	1
Pharmachem	Zinc oxide cream 25% ...	110112	1
Pharmachem	Zinc oxide oil SR 90	160413	1
Pharmachem	Zinc oxide oil SR 90	150413	1
Pharmachem	Zinc oxide oil SR 90	260412	1
Pharmachem	Zinc oxide oil SR 90	20712	1
Pharmachem	Zinc oxide oil SR 90	30712	1
Pharmachem	Zinc oxide paste, sof...	70512	1
Pharmachem	Oxytetracycline ointm...	140212	2
Pharmachem GmbH	Zinc oxide oil SR 90	61112	1
PharmaChem/Noweda	Zinc oxide oil DAC	80512	1
Pharmachem/Phönix	Zinc oxide oil SR 90	160810	1
pharmachen	Zinc oxide oil SR 90	30045100	1
Pharmachern/AHD	Zinc oxide oil SR 90	160122	1
Phoenix	Castor oil, hydrated	12071107	1
Phoenix	Castor oil, hydrated	11325205	2
Phoenix	Zinc oxide lotion, aq...	4010501	1
Phoenix	Zinc paste, soft DAB	281120	1
Phoenix (Pharmachem P...	Zinc oxide paste, sof...	191112	1
Phoenix (PKH Halle)	Methylrosanilinium ch...	4A200712	1
Phoenix (PKH Halle)	Metronidazole 10% (no...	11B251012	1
Phoenix 19.12.12	Vitamin A-palmitate (...)	12J16-N03	2
Phoenix am 19.09.2012	Coconut oil, hardened	11379505	1
Phoenix, 17.09.2012	St. John's wort oil	12076905	3
Phoenix/Apomix	Clobatesol propionate...	6A070513	1
phönix	Campher oil 10%	7/AKD57	1
Phönix	Calendula tincture (7...	13142811	9
Phönix	Calendula tincture (7...	13142803	10
Phönix	Cayenne pepper tinctu...		1
Phönix	Coal tar solution	12105-n02	1
Phönix	Coal tar solution	11B14-N04	1
Phönix	Hydrogen peroxide sol...	6313073	2
Phönix	Hydroxyethylcellulose...	13286702	1
Phönix	Hydroxyethylcellulose...	15067901	1
Phönix	Matricaria liquid ext...	12360301	1
Phönix	Opium tincture, stand...	2006413	27
Phönix	Sage leaf liquid extr...	11372206	4
Phönix	Siam benzoin tincture...	12228107	1
Phönix	St. John's wort oil	5803902	2
Phönix	St. John's wort oil	12293904	4
Phönix	Theriac	12067210	1

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Supplier	Substance	Batch	Spectra
Phönix	Thyme liquid extract	12197005	3
Phönix	Thyme tincture (70%) ...	10379114	1
Phönix	Triamcinolone acetoni...	13029801	2
Phönix	Zinc oxide lotion, aq...	11329801	3
Phönix	Zinc oxide oil DAC	1C010212	1
Phönix	Zinc oxide oil DAC	286040	1
Phönix	Zinc paste, soft DAB	15005101	1
Phönix	Castor oil, hydrated	288639	1
Phönix 11.11.2014	Food colorant green (...)	13020106	1
Phönix Gotha	Castor oil, hydrated	12H29-N04	2
Phönix Gotha	Castor oil, hydrated	12H29-N04	1
Phönix Gotha	Gentian tincture (70%...	10334601	1
Phönix Gotha	Hydrophilic metronida...	4B190413	5
Phönix Gotha	Hydrophobic triclosan...	S091201.1	1
Phönix Gotha	Hydrophobic triclosan...	561069	1
Phönix Gotha	Hydroxyethylcellulose...	11341802	1
Phönix Gotha	Hydroxyethylcellulose...	12320501	7
Phönix Gotha	Hydroxyethylcellulose...	12244003	5
Phönix Gotha	Lactic acid 80% L(+)	2002071	1
Phönix Gotha	Peanut oil, hydrated	12230701	2
Phönix Gotha	Valerian tincture (70...	11254302	1
Phönix Gotha	Vitamin A-palmitate (...)	8900521	1
Phönix Gotha	Wormwood tincture (70...	10010909	1
Phönix Gotha	Zinc oxide cream 25% ...	276963	1
Phönix Gotha	Zinc oxide lotion, aq...	259142	1
Phönix Gotha	Zinc paste, soft DAB	113381	1
Phönix Maros	Castor oil, hydrated	285801	1
Phönix Maros	Opium tincture, stand...	11008214	1
Phönix Maros	Opium tincture, stand...	7007914	2
Phönix, 16.10.2012	Coal tar solution	12E08-N01	5
phönix, 21.11.2012	Rose water	12C27-N05	2
phönix, 23.11.2012	Hydroxyethylcellulose...	24B070912	2
Phönix, 30.10.2012	Valerian tincture (70...	12113005	1
Phönix/ henry lamotte	St. John's wort oil	5442801	1
Phönix/ henry lamotte	St. John's wort oil	5171601	7
Phönix/ Maros	Opium tincture, stand...	5006613	25
Phönix/Eurho	Castor oil, hydrated	1212008-02	1
Phönix/euro	Castor oil, hydrated	1504006-02	1
Phönix/Henry Lamotte	St. John's wort oil	5540603	2
Phönix/HenryLaMotte	Zinc paste, soft DAB	56119000	1
Phönix/InfectoPharm	Hydrophobic triclosan...	S021204.1	6
Phönix/InfectoPharm	Hydrophobic triclosan...	S021205.1	4
PKH / Gehe	Hydrogen peroxide sol...	12D26-M05	1
PKH / Gehe	Hydrogen peroxide sol...	12D27-M09	1
PKH / Gehe	Hydrogen peroxide sol...	12I04-M09	1
PKH / Gehe	Hydrogen peroxide sol...	12I06-M07	2
PKH / Gehe	Hydrogen peroxide sol...	13A02-M09	3
PKH GbmH	Betamethasone valerat...	3B280213	2
PKH GbmH	Clobatesol propionate...	2A280213	1
PKH GmbH	Hydrogen peroxide sol...	487A161012	1
PKH GmbH	Zinc oxide cream 25% ...	2B080113	1
PKH GmbH/Anzag	Hydrogen peroxide sol...	485A121012	1
PKH Halle	Searing paste SR	17B211112	1
PKH Halle / Phoenix	Metronidazole 10% (no...	8B211013	1
PKH Halle / Phoenix	Searing paste SR	5B110413	2
PKH Halle / Phoenix	Searing paste SR	14B240913	4
PKH Halle/ Alliance H.	Hydroxyethylcellulose...	18B090813	1
Post-Apotheke	Food colorant green (...)	13020101	1
primavera	St. John's wort oil	12106131	1
Primavera	Aloe vera oil (with a...	8601131	1

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Supplier	Substance	Batch	Spectra
Primavera	St. John's wort oil	25508131	1
Purren Apotheke	St. John's wort oil	11205311	1
Resena/Anzag	Carotene (ca. 4m IU)	1204-3534	1
Retest	Coal tar solution	11D01-N04	1
sanacorp	Opium tincture, stand...	9005912	5
Sanacorp	Benzalkonium chloride	10190002	1
Sanacorp	Campher oil 10%	7/AKD4	1
Sanacorp	Hydrophobic triclosan...	S031105.1	1
Sanacorp	Hydroxyethylcellulose...	13190501	8
Sanacorp	Hydroxyethylcellulose...	12309303	9
Sanacorp	Hydroxyethylcellulose...	12219401	6
Sanacorp	Hydroxyethylcellulose...	12127901	2
Sanacorp	Melissa leaf tincture...	12206205	1
Sanacorp	Opium tincture, stand...	60006713	1
Sanacorp	Orange flower water	AKD34	1
Sanacorp	Peanut oil, hydrated	12298205	1
Sanacorp	St. John's wort oil	13252505	4
Sanacorp	Witch hazel leaf liqu...	13112003	1
Sanacorp	Zinc oxide lotion, aq...	AKD33	1
Sanacorp	Zinc paste DAB	13345101	8
Sanacorp	Zinc paste DAB	13201903	1
Sanacorp	Zinc paste DAB	13043401	19
Sanacorp	Zinc paste, soft DAB	274978	3
Sanacorp	Zinc paste, soft DAB	274979	1
Sanacorp, 1303.12 EK:...	Hydrophobic triclosan...	S091102.1	1
Sanacorp/ apomix	Zinc oxide oil DAC	26B190911	1
Sanacorp/ PKH Halle	Hydroxyethylcellulose...	10B200412	1
Sanacorp/ PKH Halle	Hydroxyethylcellulose...	8B050412	1
Sanacorp/Ichthyol	Methoxsalen 0.006% Co...	13D013	1
Sigmar Aldrich	Dichloroacetic acid 10%	STBC3539V	1
Sino Phyto	Hydrogen peroxide sol...	8517	1
Spinnrad/Phoenix	Witch hazel bark water	413310062	1
stumpf	Hydrogen peroxide sol...	280A060712	1
Taoasis	Aloe vera oil (with a...	110137-96542	1
Taoasis	Aloe vera oil (with a...	120247-107323	1
Taoasis	Aloe vera oil (with a...	130237-111659	1
Taoasis	Aloe vera oil (with a...	130501-112371	1
Taoasis	Aloe vera oil (with a...	111208-105327	1
Taoasis	Aloe vera oil (with a...	120247-106498	1
Taoasis	Arnica oil, fat	7525-113064	1
Taoasis	Arnica oil, fat	7360-112511	1
Taoasis	Arnica oil, fat	7360-111459	1
Taoasis	Arnica oil, fat	7360-111366	1
Taoasis	Calendula oil, fat	119426-108734	1
Taoasis	Calendula oil, fat	119943-110316	1
Taoasis	Siam benzoin	541389-111081	1
Taoasis	St. John's wort oil	123212-111876	1
Taoasis	St. John's wort oil	145646-103095	1
Taoasis	St. John's wort oil	123212-110835	1
Taoasis	St. John's wort oil	12312-109683	1
Taoasis GmbH	St. John's wort oil	150822-107470	1
Teofarma	Arnica tincture (70%)...	144301	2
Wasserfuhr	Zinc paste DAB	12169401	1

Appendix D: Requirements of validation

In order to ensure adherence to the safe scientific status, the individual methods for manufacturing and testing must be validated under certain circumstances (compare § 34 para. 1 no. 3, § 35 para. 1 no. 4 and para. 4 sentence 1 no. 2 b, para. 6 sentence 3 *ApoBetrO* [Pharmacies Rules and Regulations]). The *ApoBetrO* [Pharmacies Rules and Regulations] incorporates a legal definition in § 1 a para. 16 (quotation translated):

“Validation is the provision of documented proof which with a high degree of safety documents that, via a specific process or standard work process, a medicinal product is manufactured and tested, which is in accordance with previously determined quality features.”

Validation documentation can be used to prove that methods or devices which are not described in the Pharmacopoeia within the meaning of § 6 para. 1 sentence 3 *ApBetrO* [Pharmacies Rules and Regulations] achieve the same results as those in the Pharmacopoeia. On the other hand, with the requirements of the demanded validation it must be observed whether the respective testing method is already incorporated in the Pharmacopoeia.

NIR spectroscopy as a general testing method need not be validated in accordance with the express ruling in the *Ph. Eur. Section 1.1* [3], as it is already described in *Section 2.2.40* of the *Ph. Eur.* as an area of application for the identification of raw materials.

However, a special validation requirement exists for the reference database. This requirement is met with the existing document. Further requirements or rules as to how this proof must be furnished do not exist. It is required that the processes guarantee the same results as the methods and devices in the Pharmacopoeia [17].

Carrying out identity tests with *Apo-Ident* is therefore also possible if the NIR spectroscopy process is not required in the Pharmacopoeia monograph of the substance for identity testing. All NIR analyses with *Apo-Ident* prove several, often all molecule groups and are therefore comparable with a series of individual, targeted chemical proofs [4]. Therefore, the identity proof with *Apo-Ident* replaces the monograph test series (with two or more test combinations).

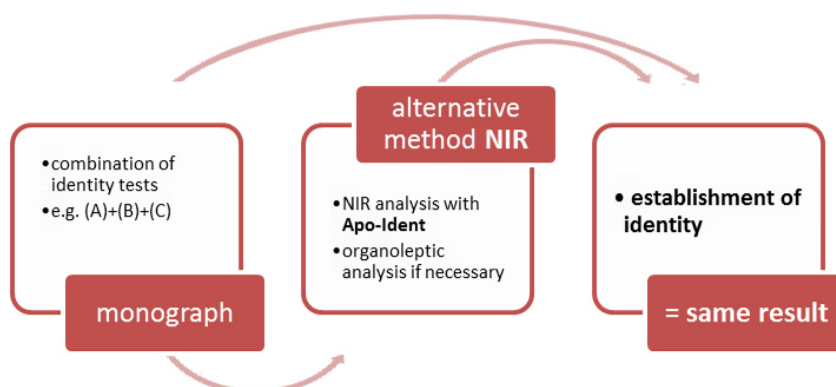


Figure 2: The combination of tests of the monograph is replaced by the alternative method NIR spectroscopy using *Apo-Ident*. This is permissible because both test procedures result in the establishment of the identity of the raw material.

With this validation documentation, proof is furnished that identical results are achieved with *Apo-Ident* and Pharmacopoeia methods, i.e. confirmation of the identity of the raw material [2].

Appendix E: Conformity of Apo-Ident with the European pharmacopeia

According to *Ph. Eur. Section 2.2.40*, NIR spectroscopy is basically suitable for: “Identification of agents, excipients, dosage forms, intermediate manufacturing products, chemical raw materials and packaging materials” ([3], quotation translated).

The fact that *Apo-Ident* meets the further criteria of the European Pharmacopoeia under the headings in *Section 2.2.40*

- Apparatus
- Measurement methods
- Sample preparation and presentation
- Testing the functionality of the instrument
- Identification and characterisation (qualitative analysis)
- Quantitative analysis
- Ongoing model evaluation
- Transfer of databases
- Data storage

can be proven based on the *HiperScan GmbH* documentation of “Meeting 2.2.40 *Ph. Eur.* by *Apo-Ident*” [4].

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